



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 04:57 PM JST

PDB ID : 7XNX / pdb_00007xnx
EMDB ID : EMD-33329
Title : High resolution cry-EM structure of the human 80S ribosome from
SNORD127+/+ Kasumi-1 cells
Authors : Cheng, J.; Beckmann, R.
Deposited on : 2022-04-30
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

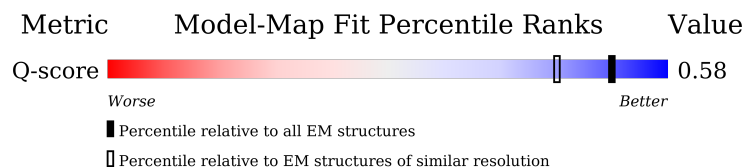
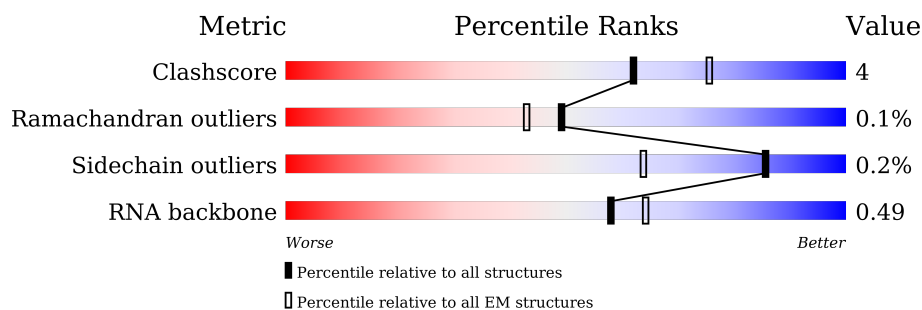
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



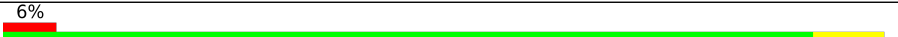
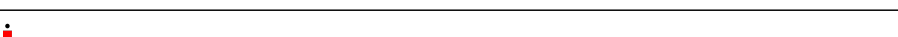
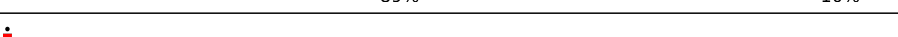
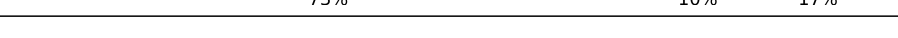
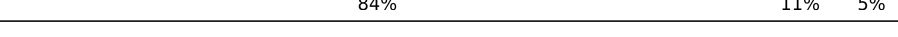
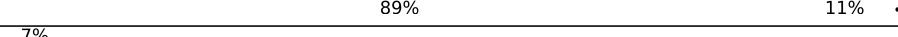
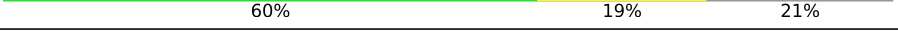
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L1	5070	
2	L2	121	
3	L3	157	

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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	282	

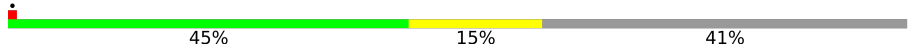
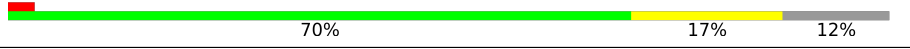
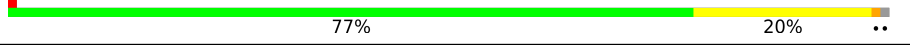
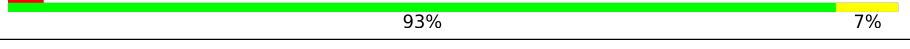
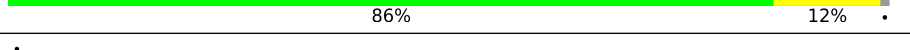
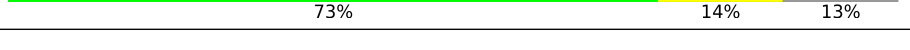
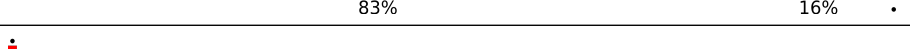
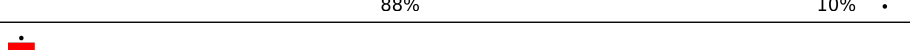
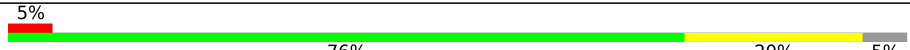
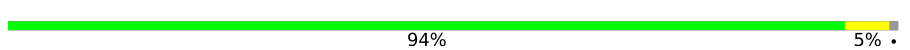
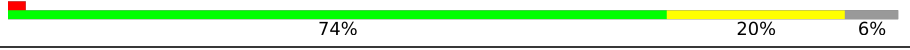
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Mol	Chain	Length	Quality of chain
28	La	282	
29	Lb	159	
30	Lc	115	
31	Ld	125	
32	Le	135	
33	Lf	110	
34	Lg	117	
35	Lh	123	
36	Li	105	
37	Lj	97	
38	Lk	70	
39	Ll	51	
40	Lm	128	
41	Ln	25	
42	Lo	106	
43	Lp	92	
44	Lr	137	
45	S2	1869	
46	SA	295	
47	SB	264	
48	SD	243	
49	SE	263	
50	SF	204	
51	SH	194	
52	SI	208	

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Mol	Chain	Length	Quality of chain
53	SK	165	
54	SL	158	
55	SP	145	
56	SQ	146	
57	SR	135	
58	SS	152	
59	ST	145	
60	SU	119	
61	SV	83	
62	SX	143	
63	Sa	115	
64	Sc	69	
65	Sd	56	
66	Sg	317	
67	SC	293	
68	SG	249	
69	SJ	194	
70	SM	132	
71	SN	151	
72	SO	151	
73	SW	130	
74	SY	133	
75	SZ	125	
76	Sb	84	
77	Se	59	

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Mol	Chain	Length	Quality of chain
78	CE	133	8%48%6%46%
78	Sf	133	39%7%54%
79	CC	75	37%67%48%15%

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 218434 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	3773	Total	C	N	O	P	0	0
			80211	35727	14590	26122	3772		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	220	Total	C	N	O	S	0	0
			1765	1136	334	291	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	227	Total	C	N	O	S	0	0
			1835	1171	353	307	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein L10 isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	169	Total	C	N	O	S	0	0
			1353	856	253	238	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		
28	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 31 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 33 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 34 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 35 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 36 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 37 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 40 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 41 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	103	Total	C	N	O	S	0	0
			843	529	172	136	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 45 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S2	1740	Total	C	N	O	P	0	0
			36959	16515	6600	12105	1739		

- Molecule 46 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

- Molecule 47 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 48 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 49 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 50 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 51 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 52 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 53 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 54 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 55 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 56 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 57 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 58 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 59 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 60 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 61 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 62 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 63 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 64 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 65 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 68 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 70 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 71 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 72 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 73 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SY	125	Total	C	N	O	S	0	0
			1022	645	200	172	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 76 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		
78	CE	72	Total	C	N	O		0	0
			603	395	105	103			

- Molecule 79 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	CC	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	L1	264	Total	Mg	0
			264	264	
80	L2	3	Total	Mg	0
			3	3	
80	L3	5	Total	Mg	0
			5	5	
80	LA	1	Total	Mg	0
			1	1	
80	LC	2	Total	Mg	0
			2	2	
80	LI	1	Total	Mg	0
			1	1	
80	LN	1	Total	Mg	0
			1	1	
80	LP	1	Total	Mg	0
			1	1	
80	LV	1	Total	Mg	0
			1	1	
80	Le	1	Total	Mg	0
			1	1	
80	Lf	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	Lg	1	Total 1	Mg 1	0
80	S2	135	Total 135	Mg 135	0
80	Sd	1	Total 1	Mg 1	0
80	SG	1	Total 1	Mg 1	0
80	SJ	1	Total 1	Mg 1	0
80	CC	1	Total 1	Mg 1	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
81	L1	12	Total 12	K 12	0

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	Lg	1	Total 1	Zn 1	0
82	Lj	1	Total 1	Zn 1	0
82	Lm	1	Total 1	Zn 1	0
82	Lo	1	Total 1	Zn 1	0
82	Lp	1	Total 1	Zn 1	0
82	Sa	1	Total 1	Zn 1	0
82	Sd	1	Total 1	Zn 1	0
82	Sb	1	Total 1	Zn 1	0
82	Sf	1	Total 1	Zn 1	0

- Molecule 83 is water.

Mol	Chain	Residues	Atoms	AltConf
83	L1	762	Total O 762 762	0
83	L2	3	Total O 3 3	0
83	L3	6	Total O 6 6	0
83	LA	6	Total O 6 6	0
83	LB	3	Total O 3 3	0
83	LC	13	Total O 13 13	0
83	LD	1	Total O 1 1	0
83	LI	2	Total O 2 2	0
83	LL	1	Total O 1 1	0
83	LN	1	Total O 1 1	0
83	LP	1	Total O 1 1	0
83	LR	1	Total O 1 1	0
83	LX	2	Total O 2 2	0
83	LY	2	Total O 2 2	0
83	La	8	Total O 8 8	0
83	Lb	1	Total O 1 1	0
83	Le	2	Total O 2 2	0
83	Lg	2	Total O 2 2	0
83	Lj	4	Total O 4 4	0
83	Ll	2	Total O 2 2	0
83	Lo	1	Total O 1 1	0
83	S2	10	Total O 10 10	0

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Mol	Chain	Residues	Atoms		AltConf
83	SX	1	Total	O	0
			1	1	
83	CE	1	Total	O	0
			1	1	

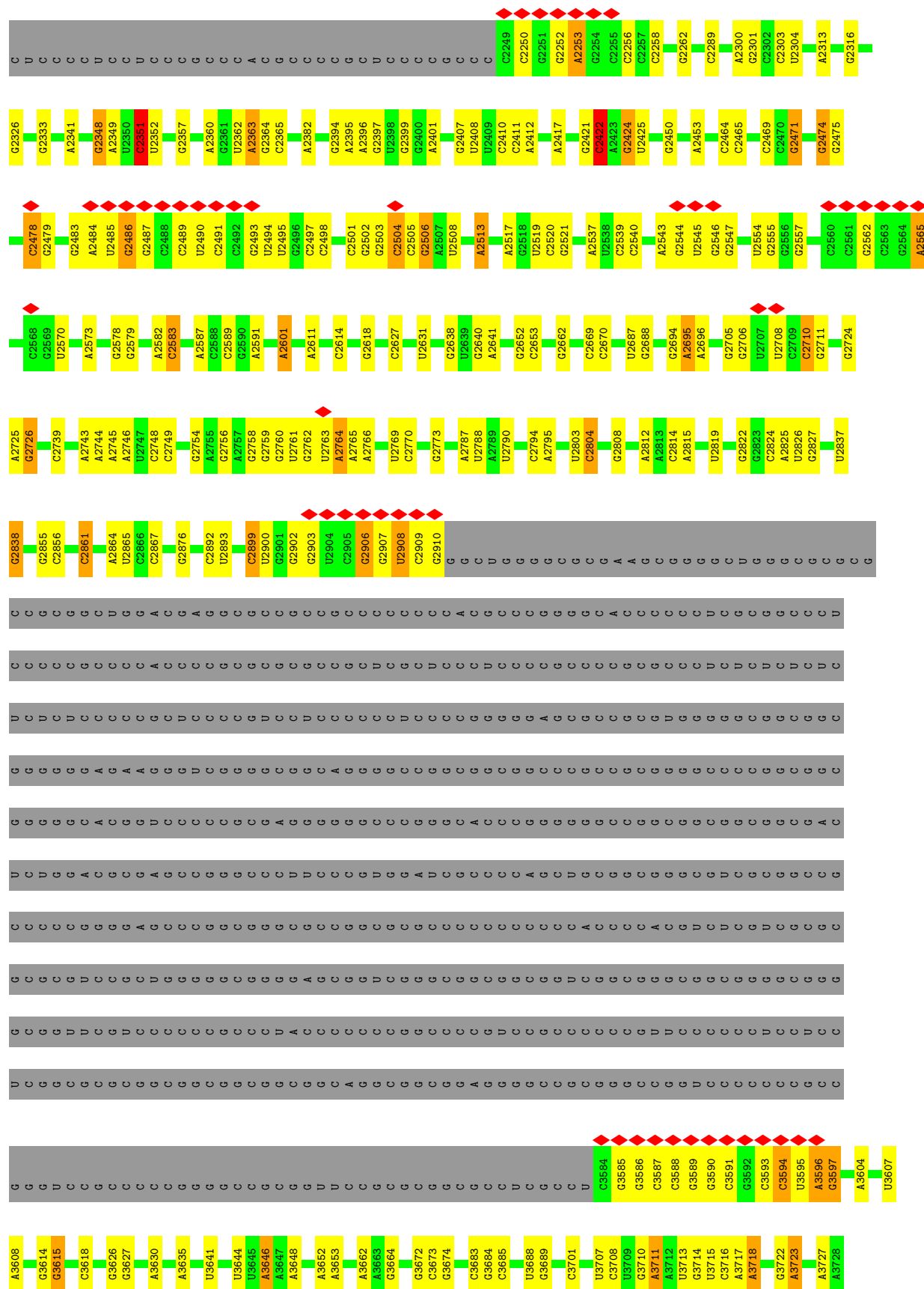
3 Residue-property plots [i](#)

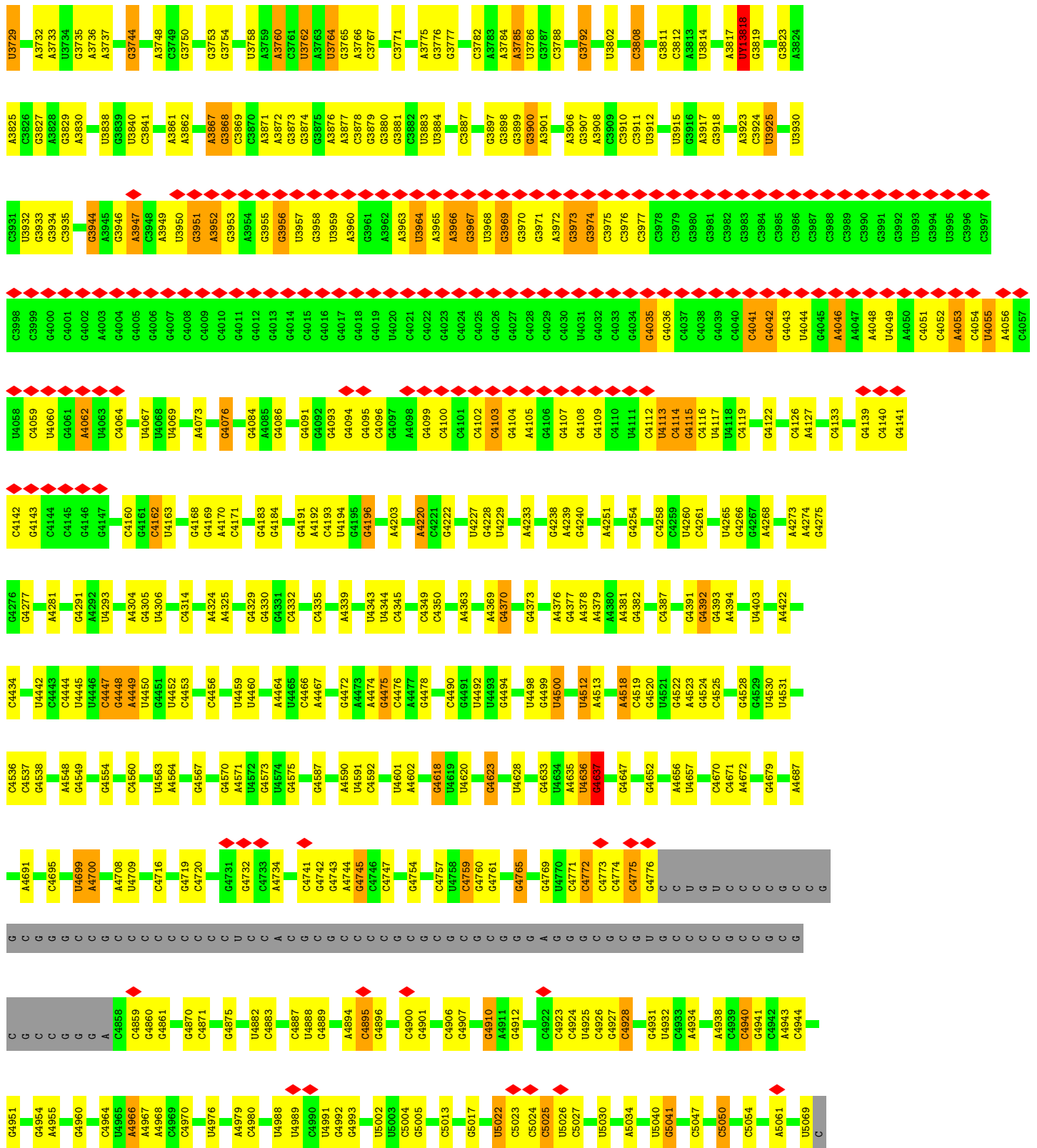
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 28S rRNA



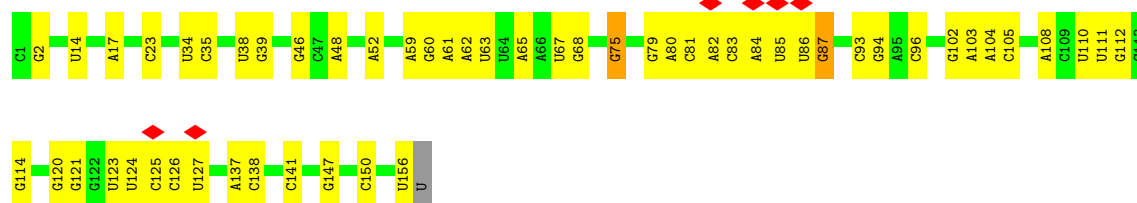




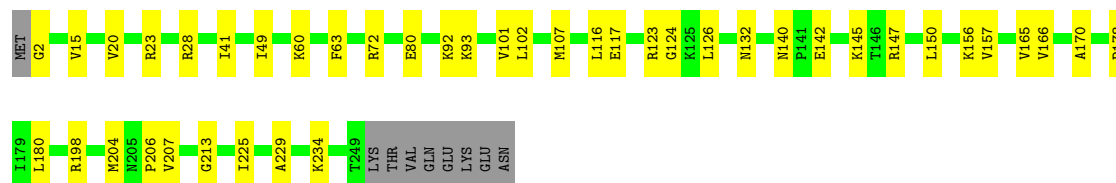
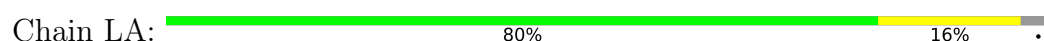




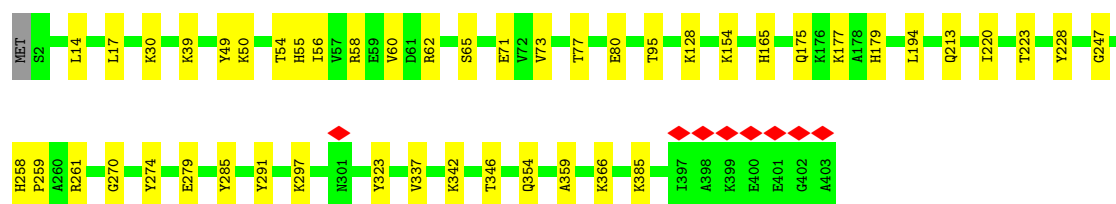
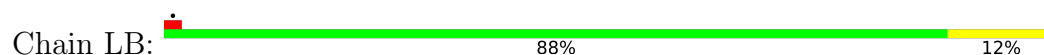
- Molecule 3: 5.8S rRNA



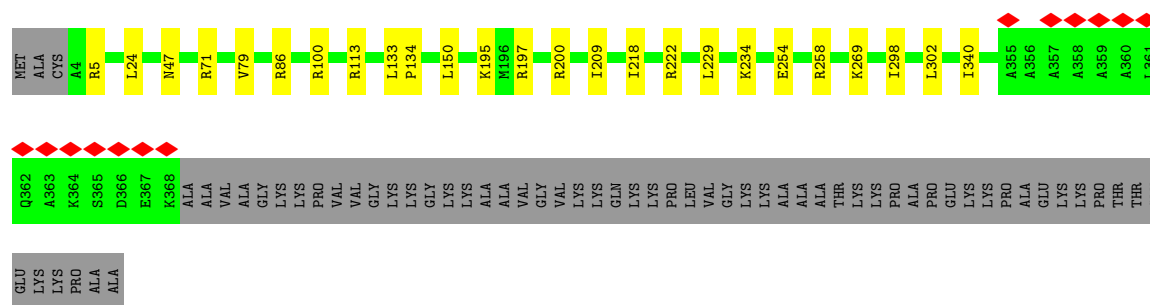
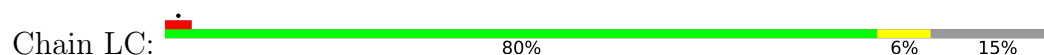
- Molecule 4: 60S ribosomal protein L8



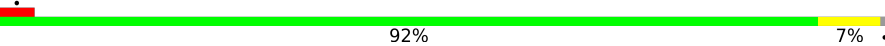
- Molecule 5: 60S ribosomal protein L3

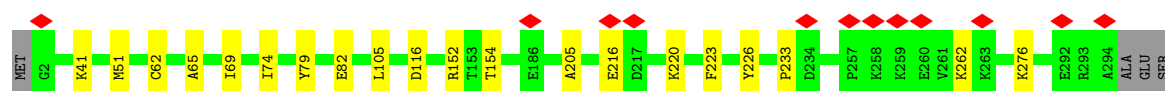


- Molecule 6: 60S ribosomal protein L4



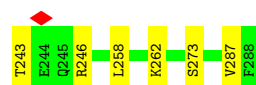
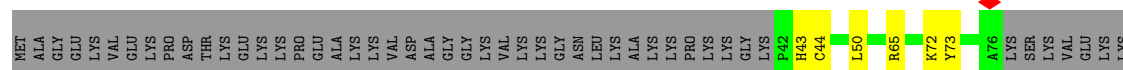
- Molecule 7: 60S ribosomal protein L5

Chain LD:  92% 7%



• Molecule 8: 60S ribosomal protein L6

Chain LE:  66% 10% 24%



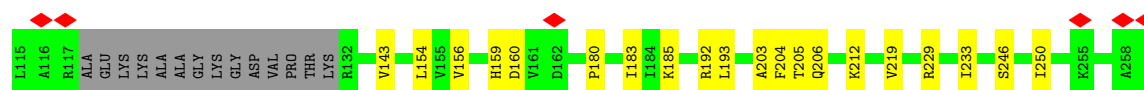
• Molecule 9: 60S ribosomal protein L7

Chain LF:  82% 8% 9%



• Molecule 10: 60S ribosomal protein L7a

Chain LG:  6% 70% 15% 15%

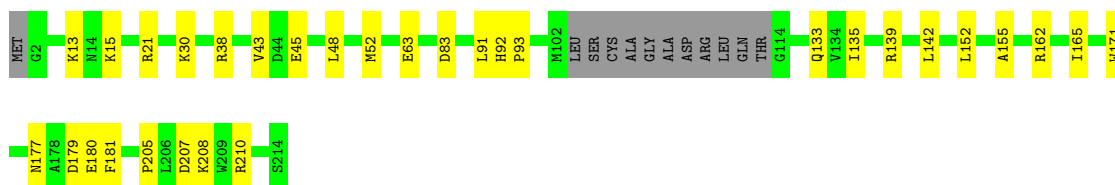
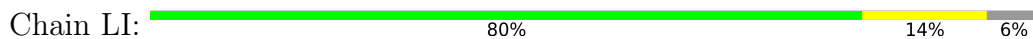


• Molecule 11: 60S ribosomal protein L9

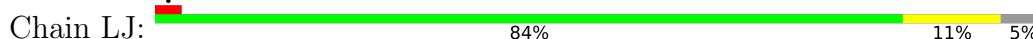
Chain LH:  84% 15%



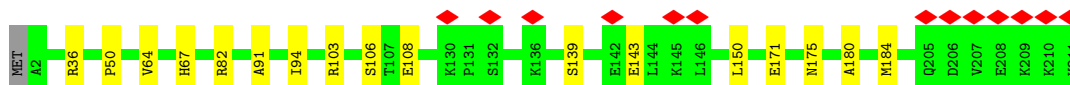
- Molecule 12: Ribosomal protein L10 isoform A



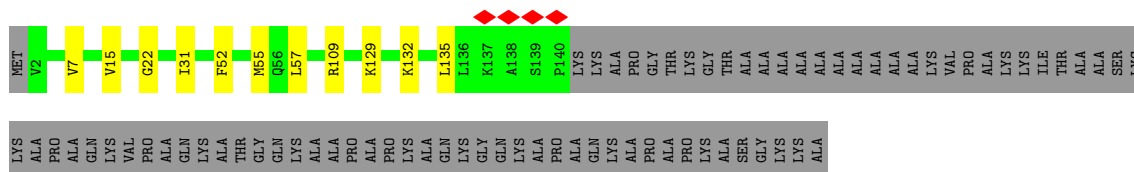
- Molecule 13: 60S ribosomal protein L11



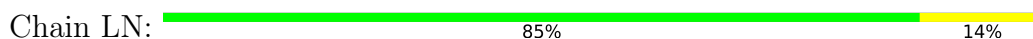
- Molecule 14: 60S ribosomal protein L13



- Molecule 15: 60S ribosomal protein L14



- Molecule 16: 60S ribosomal protein L15

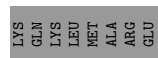
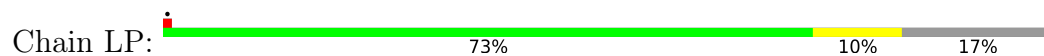


- Molecule 17: 60S ribosomal protein L13a

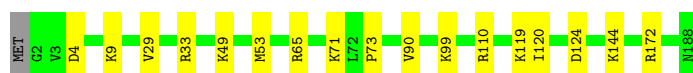




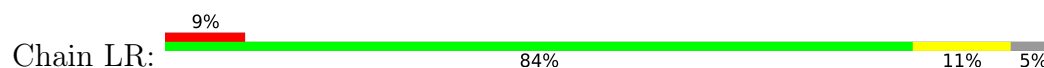
- Molecule 18: 60S ribosomal protein L17



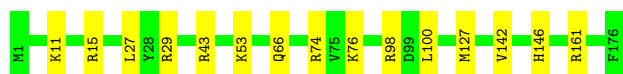
- Molecule 19: 60S ribosomal protein L18



- Molecule 20: 60S ribosomal protein L19



- Molecule 21: 60S ribosomal protein L18a



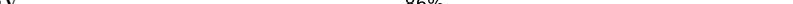
- Molecule 22: 60S ribosomal protein L21

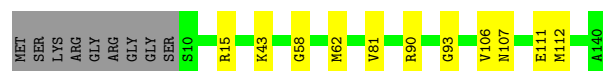


- Molecule 23: 60S ribosomal protein L22

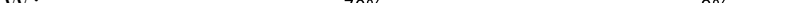


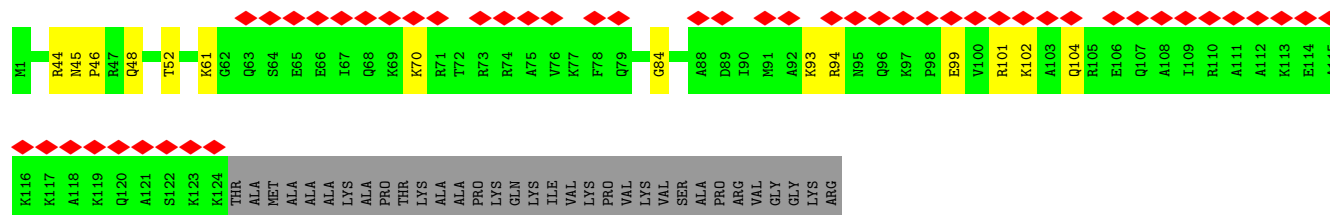
- Molecule 24: 60S ribosomal protein L23

Chain LV: 



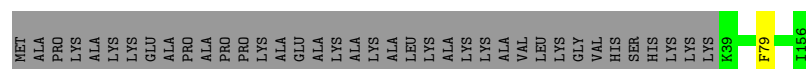
- Molecule 25: 60S ribosomal protein L24

Chain LW: 



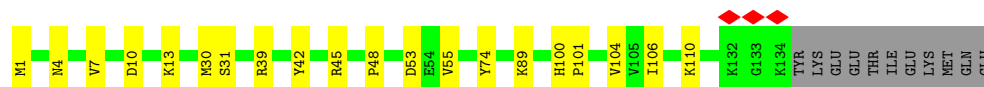
- Molecule 26: 60S ribosomal protein L23a

Chain LX:  75% 24%

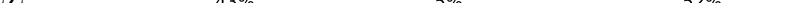


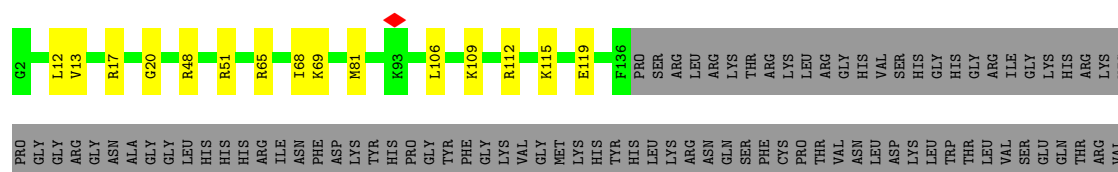
- Molecule 27: 60S ribosomal protein L26

Chain LY: 79% 14% 8%



- Molecule 28: 60S ribosomal protein L27

Chain LZ: 



ASN
ALA
ALA
LYS
MET
LYS
ASN
LYS
THR
GLY
ALA
ALA
PRO
PRO
ILE
ASP
VAL
VAL
ARG
SER
GLY
TYR
TYR
LYS
VAL
VAL
GLY
LYS
GLY
LYS
LEU
PRO
LYS
GLN
PRO
VAL
ILE
VAL
LYS
ALA
PHE
PHE
SER
SER
ARG
ARG
ALA
GLU
GLU
LYS
ILE
LYS
LYS
SER
VAL
GLY
GLY
CYS
VAL
VAL
VAL
LYS
ALA

• Molecule 28: 60S ribosomal protein L27

Chain La: 45% 7% 48%

GLY
LYS
PHE
MET
LYS
LYS
PRO
GLY
LYS
VAL
VAL
VAL
VAL
VAL
ALA
GLY
ARG
TYR
ASN
TYR
HIS
SER
GLY
ARG
LYS
ALA
VAL
VAL
ILE
VAL
LYS
ASN
ILE
ILE
ASP
PRO
LEU
ASP
GLY
GLY
THR
SER
VAL
VAL
ARG
PRO
LYS
TYR
SER
ASP
VAL
PHE
HIS
LEU
VAL
ASP
PRO
ALA
GLY
ILE
ASP
LYS
ARG
ARG
TYR
PRO
ALA
LYS
VAL
THR
VAL
MET
GLY
LYS
LYS
ARG

ILE
ALA
LYS
ARG
SER
LYS
ILE
LYS
SER
PHE
PHE
GLN
LYS
VAL
TYR
ASN
TYR
HIS
SER
LEU
MET
PRO
THR
ARG
TYR
SER
VAL
ASP
VAL
ILE
PRO
LEU
ASP
LYS
THR
VAL
VAL
ASN
LYS
ASP
VAL
PHE
HIS
LEU
ASP
PRO
ALA
LEU
LYS
ARG
LYS
ALA
ARG
ARG
LYS
VAL
ALA
LYS
PHE
GLU
GLU
ARG

TYR
LYS
THR
THR
ASN
LYS
ASN
LYS
TRP
PHE
PHE
GLN
LYS
ARG
PHE
P2
S3
R4
K7
V56
P71
T72
V73
N74
L75
L78
W79
T80
L81
V82
S83
E84
R87
K94
I101
Y108
G115
K116
L117
R132
E135
K136
A148

• Molecule 29: 60S ribosomal protein L29

Chain Lb: 9% 62% 7% 31%

MET
A2
K3
K23
D36
R41
R44
H49
A62
M65
S66
A67
A69
E70
A71
I72
K73
A74
L75
V76
LYS
PRO
LYS
GLU
VAL
LYS
PRO
LYS
ILE
PRO
LYS
GLY
V89
G115
L116
R117
L118
C119
K122
LYS
LYS
ALA
ALA
LYS
LYS
LYS
LYS
ASP
GLN
THR

LYS
ALA
GLN
ALA
ALA
LYS
PRO
ALA
ALA
PRO
LYS
LYS
THR
GLN
ALA
PRO
LYS
SER
GLU

• Molecule 30: 60S ribosomal protein L30

Chain Lc: 73% 12% 15%

MET
VAL
ALA
ALA
LYS
LYS
THR
LYS
K9
V28
T34
L35
K36
M37
I38
R39
Q40
A43
I47
L48
K57
Y63
L94
A95
I96
I97
R106
SER
MET
PRO
GLU
GLN
THR
GLY
GLU
LYS

• Molecule 31: 60S ribosomal protein L31

Chain Ld: 6% 81% 5% 14%

MET
ALA
PRO
ALA
LYS
LYS
GLY
GLY
LYS
LYS
LYS
GLY
ARG
SER
ALA
ALA
ILE
N18
E19
I29
I33
V62
R63
I64
L68
E94
D95
E96
D97
S98
T104
D123
E124
ASN

• Molecule 32: 60S ribosomal protein L32

Chain Le: 84% 11% 5%

MET
A2
D26
W35
P38
R46
P56
E84
V87
L88
L89
N92
V103
S104
R108
L118
N124
A127
R128
L129
ARG
SER
GLU
GLU
ASN
GLU

• Molecule 33: 60S ribosomal protein L35a

Chain Lf:  92% 7%



- Molecule 34: 60S ribosomal protein L34

Chain Lg:  85% 13%

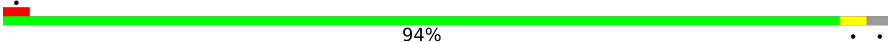


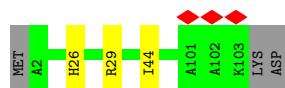
- Molecule 35: 60S ribosomal protein L35

Chain Lh:  85% 14%



- Molecule 36: 60S ribosomal protein L36

Chain Li:  94%



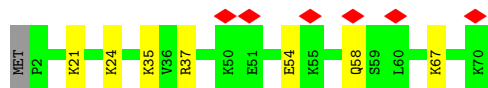
- Molecule 37: 60S ribosomal protein L37

Chain Lj:  77% 11% 11%



- Molecule 38: 60S ribosomal protein L38

Chain Lk:  9% 89% 10%

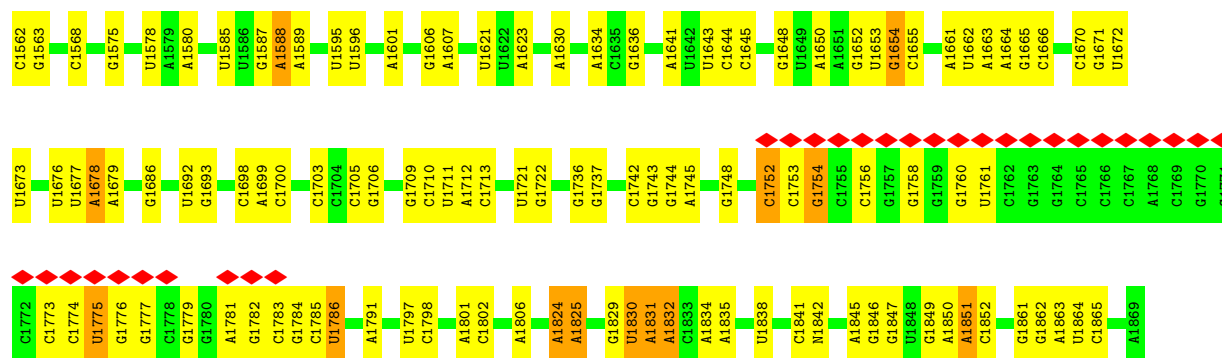


- Molecule 39: 60S ribosomal protein L39

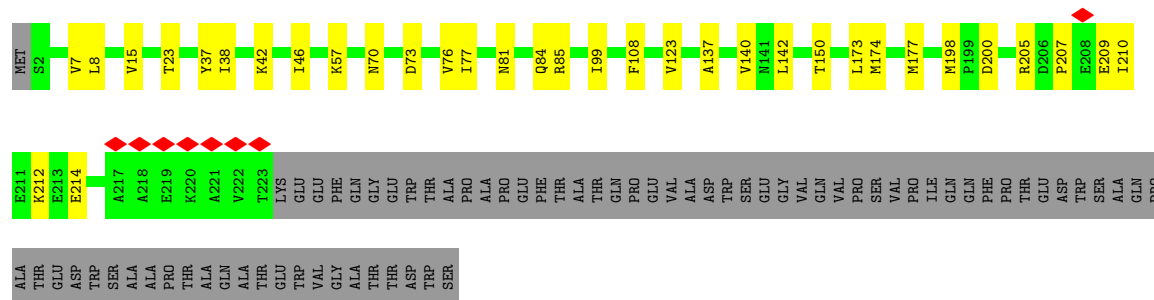
Chain Ll:  86% 12%



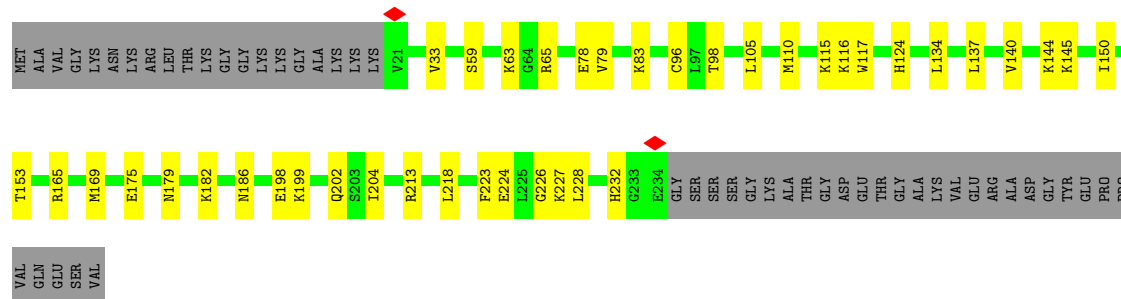




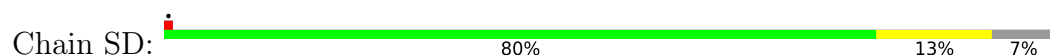
• Molecule 46: 40S ribosomal protein SA



• Molecule 47: 40S ribosomal protein S3a

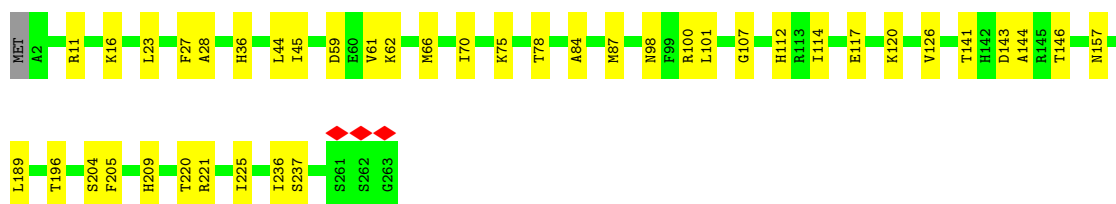


• Molecule 48: 40S ribosomal protein S3



• Molecule 49: 40S ribosomal protein S4, X isoform

Chain SE:  84% 16%



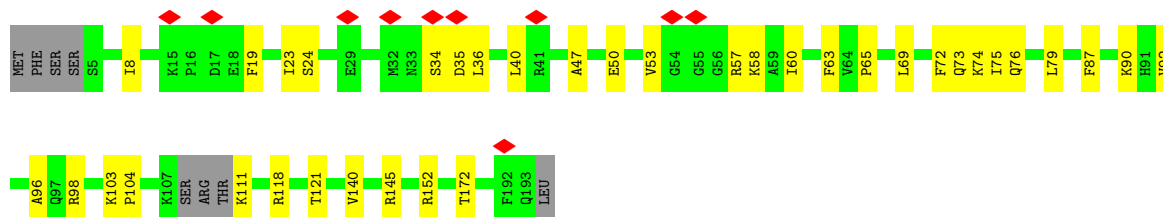
- Molecule 50: 40S ribosomal protein S5

Chain SF:  75% 15% 10%



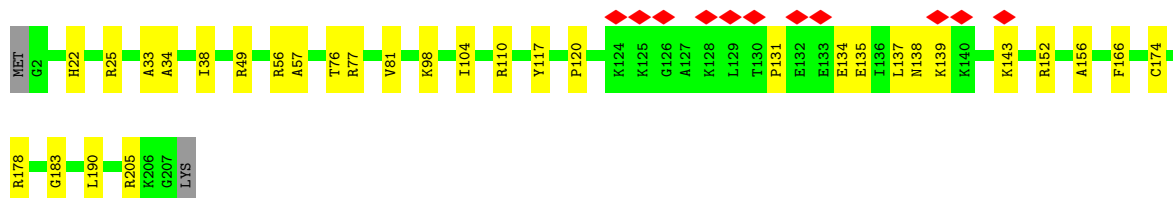
- Molecule 51: 40S ribosomal protein S7

Chain SH:  5% 77% 19%



- Molecule 52: 40S ribosomal protein S8

Chain SI:  5% 84% 15%



- Molecule 53: 40S ribosomal protein S10

Chain SK:  45% 15% 41%



PRO ALA ARG LEU THR ARG GLY GLU ALA ASP ARG ASP THR TYR ARG ARG SER ALA VAL PRO PRO GLY ALA ASP LYS LYS ALA GLU ALA GLY ALA GLY ALA GLY THR PHE GLU PHE GLN PHE ARG GLY GLN PRO PRO GLN

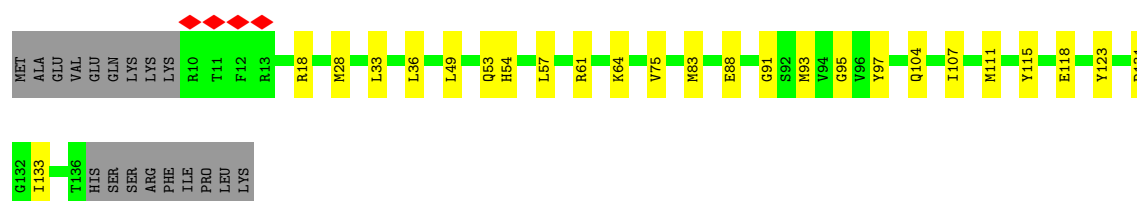
- Molecule 54: 40S ribosomal protein S11

Chain SL:  82% 9% 9%



- Molecule 55: 40S ribosomal protein S15

Chain SP:  70% 17% 12%

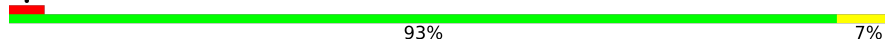


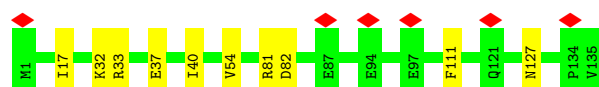
- Molecule 56: 40S ribosomal protein S16

Chain SQ:  77% 20% 3%



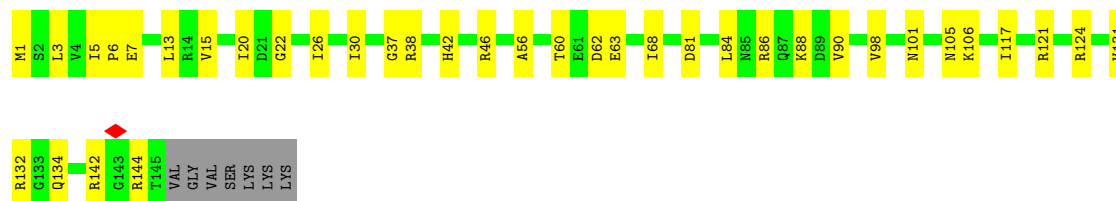
- Molecule 57: 40S ribosomal protein S17

Chain SR:  93% 7%



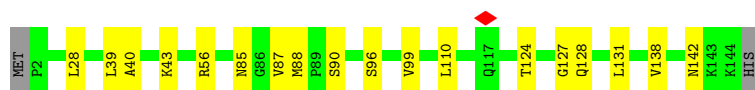
- Molecule 58: 40S ribosomal protein S18

Chain SS:  71% 24% 5%

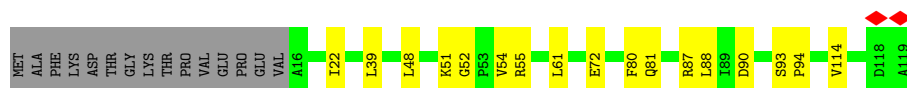
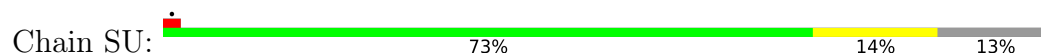


- Molecule 59: 40S ribosomal protein S19

Chain ST:  86% 12% 2%



- Molecule 60: 40S ribosomal protein S20



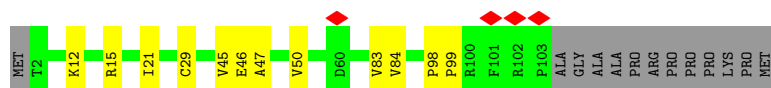
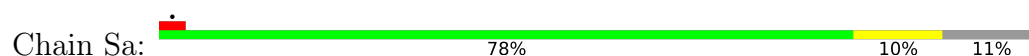
- Molecule 61: 40S ribosomal protein S21



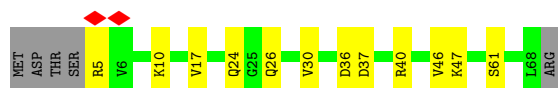
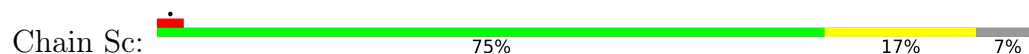
- Molecule 62: 40S ribosomal protein S23



- Molecule 63: 40S ribosomal protein S26



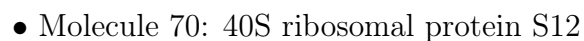
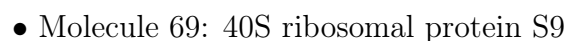
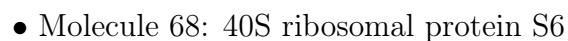
- Molecule 64: 40S ribosomal protein S28

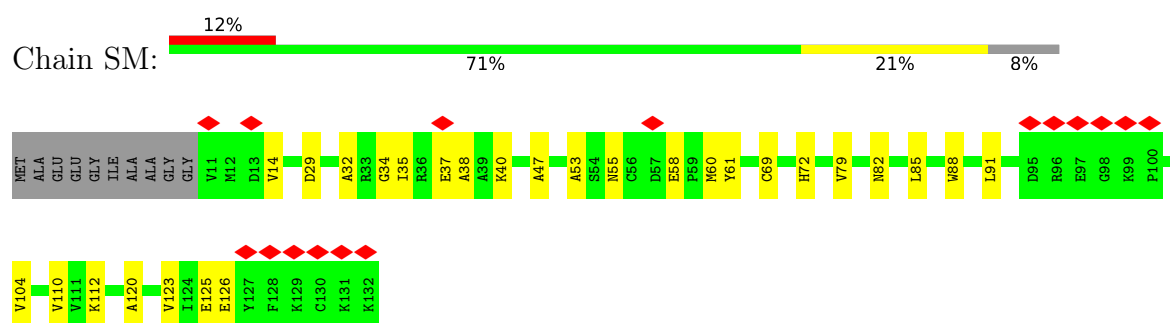


- Molecule 65: 40S ribosomal protein S29

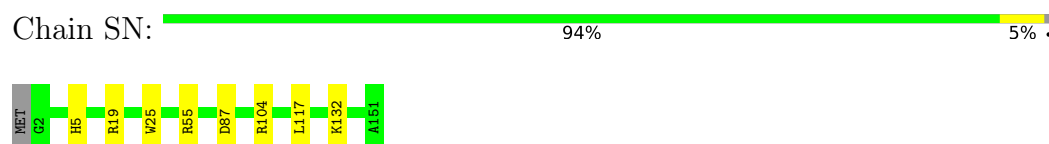


- Molecule 66: Receptor of activated protein C kinase 1

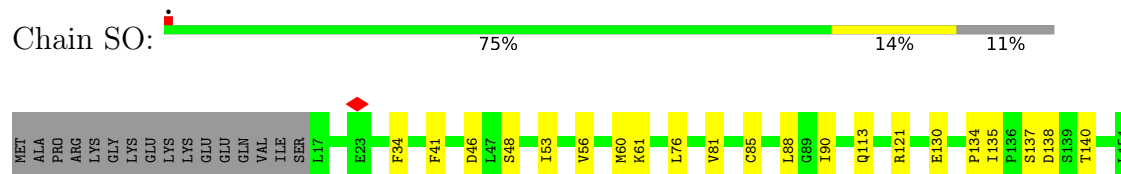




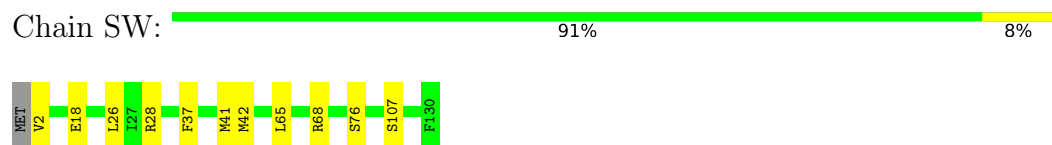
- Molecule 71: 40S ribosomal protein S13



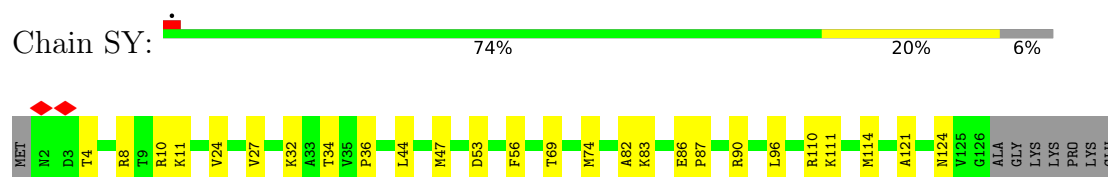
- Molecule 72: 40S ribosomal protein S14



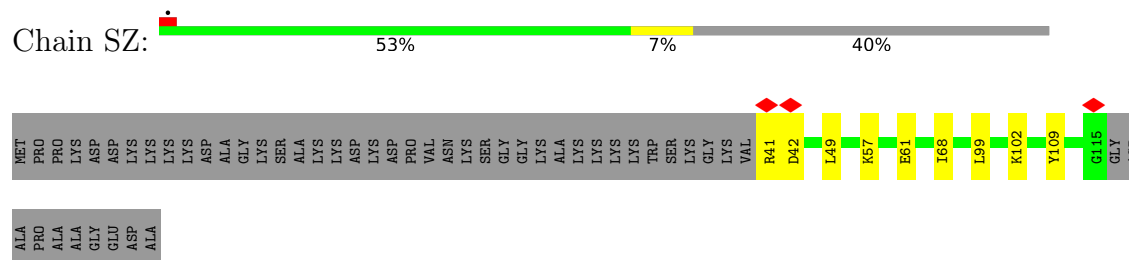
- Molecule 73: 40S ribosomal protein S15a



- Molecule 74: 40S ribosomal protein S24

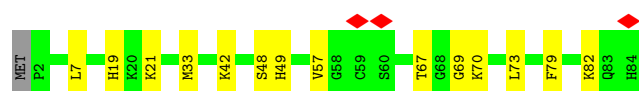


- Molecule 75: 40S ribosomal protein S25



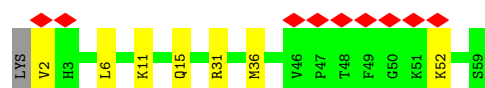
- Molecule 76: 40S ribosomal protein S27

Chain Sb:  82% 17% .



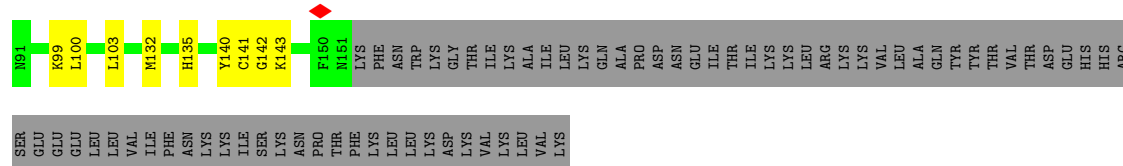
- Molecule 77: 40S ribosomal protein S30

Chain Se:  15% 86% 12% .

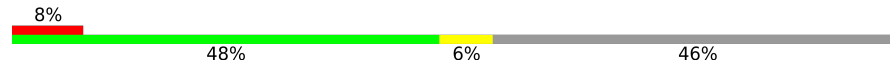


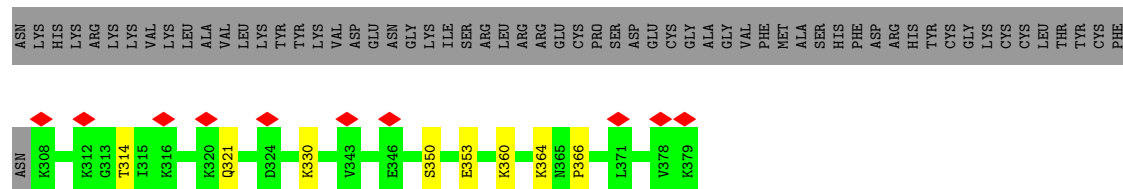
- Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  39% 7% 54%



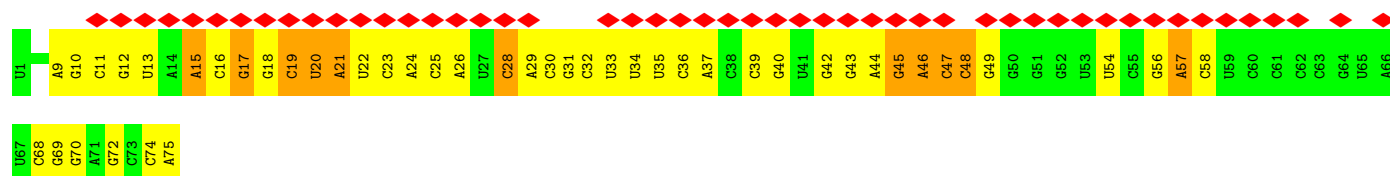
- Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain CE:  8% 48% 6% 46%



- Molecule 79: tRNA

Chain CC:  37% 67% 48% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	48.809	Depositor
Minimum map value	-19.709	Depositor
Average map value	0.030	Depositor
Map value standard deviation	1.171	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, 5MC, UY1, OMC, 1MA, B8T, PSU, A2M, MA6, 6MZ, K, UR3, ZN, MG, M7A, JMH, 4AC, OMG, 2MG, 5MU, B8N, B8H, OMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L1	0.27	2/87525 (0.0%)	0.37	1/136449 (0.0%)
2	L2	0.22	0/2858	0.32	0/4455
3	L3	0.25	0/3653	0.33	0/5691
4	LA	0.35	0/1936	0.66	0/2596
5	LB	0.27	0/3306	0.57	0/4424
6	LC	0.29	0/2962	0.55	0/3977
7	LD	0.20	0/2428	0.43	0/3252
8	LE	0.21	0/1799	0.52	0/2414
9	LF	0.30	0/1905	0.51	0/2539
10	LG	0.23	0/1866	0.50	0/2511
11	LH	0.22	0/1537	0.46	0/2066
12	LI	0.30	0/1677	0.51	0/2237
13	LJ	0.19	0/1376	0.52	0/1840
14	LL	0.24	0/1732	0.52	0/2315
15	LM	0.24	0/1161	0.53	0/1554
16	LN	0.32	0/1746	0.55	0/2338
17	LO	0.27	0/1682	0.50	1/2250 (0.0%)
18	LP	0.23	0/1268	0.50	0/1701
19	LQ	0.25	0/1537	0.49	0/2052
20	LR	0.28	0/1582	0.47	0/2091
21	LS	0.25	0/1501	0.45	0/2013
22	LT	0.25	0/1326	0.49	0/1770
23	LU	0.26	0/839	0.74	2/1126 (0.2%)
24	LV	0.25	0/993	0.52	0/1332
25	LW	0.21	0/1030	0.49	0/1364
26	LX	0.20	0/984	0.43	0/1323
27	LY	0.21	0/1132	0.46	0/1504
28	LZ	0.25	0/1129	0.55	1/1507 (0.1%)
28	La	0.28	0/1191	0.57	0/1591
29	Lb	0.24	0/889	0.54	0/1175
30	Lc	0.26	0/774	0.52	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Ld	0.23	0/903	0.48	0/1216
32	Le	0.26	0/1071	0.55	0/1429
33	Lf	0.26	0/895	0.54	0/1198
34	Lg	0.25	0/916	0.46	0/1220
35	Lh	0.24	0/1023	0.43	1/1351 (0.1%)
36	Li	0.19	0/843	0.42	0/1115
37	Lj	0.33	0/720	0.61	0/952
38	Lk	0.24	0/575	0.57	0/761
39	Ll	0.26	0/454	0.50	0/599
40	Lm	0.20	0/435	0.44	0/575
41	Ln	0.24	0/231	0.43	0/294
42	Lo	0.22	0/845	0.44	0/1113
43	Lp	0.26	0/718	0.52	0/953
44	Lr	0.23	0/1017	0.46	0/1364
45	S2	0.23	1/39961 (0.0%)	0.34	0/62247
46	SA	0.23	0/1784	0.47	0/2424
47	SB	0.24	0/1765	0.51	0/2362
48	SD	0.19	0/1793	0.44	0/2414
49	SE	0.21	0/2118	0.50	0/2849
50	SF	0.20	0/1481	0.50	0/1988
51	SH	0.54	0/1519	0.74	0/2033
52	SI	0.24	0/1715	0.54	0/2287
53	SK	0.20	0/851	0.52	0/1147
54	SL	0.22	0/1202	0.42	0/1606
55	SP	0.21	0/1065	0.55	0/1423
56	SQ	0.26	0/1160	0.66	2/1553 (0.1%)
57	SR	0.28	1/1105 (0.1%)	0.43	0/1484
58	SS	0.21	0/1216	0.57	0/1628
59	ST	0.19	0/1131	0.46	0/1515
60	SU	0.45	0/831	0.68	0/1115
61	SV	0.32	0/643	0.53	0/860
62	SX	0.22	0/1116	0.52	2/1490 (0.1%)
63	Sa	0.28	0/836	0.62	0/1121
64	Sc	0.23	0/508	0.55	0/680
65	Sd	0.20	0/470	0.56	0/623
66	Sg	0.19	0/2493	0.56	0/3394
67	SC	0.24	0/1762	0.50	0/2381
68	SG	0.26	0/1946	0.51	0/2590
69	SJ	0.23	0/1550	0.48	0/2069
70	SM	0.27	0/950	0.71	2/1275 (0.2%)
71	SN	0.21	0/1232	0.41	0/1656
72	SO	0.23	0/1023	0.51	0/1372
73	SW	0.23	0/1051	0.50	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	SY	0.20	0/1039	0.49	0/1381
75	SZ	0.17	0/604	0.49	0/810
76	Sb	0.19	0/665	0.45	0/891
77	Se	0.14	0/465	0.38	0/612
78	CE	0.16	0/613	0.48	0/819
78	Sf	0.17	0/507	0.55	0/673
79	CC	0.15	0/1773	0.34	0/2759
All	All	0.25	4/229913 (0.0%)	0.43	12/337572 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	LP	0	1
56	SQ	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SR	127	ASN	CA-CB	6.44	1.62	1.53
1	L1	4523	A2M	O3'-P	5.54	1.61	1.56
1	L1	3785	A2M	O3'-P	5.37	1.61	1.56
45	S2	668	A2M	O3'-P	5.09	1.61	1.56

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Lh	87	LYS	CB-CA-C	-5.96	109.69	116.54
17	LO	110	PRO	N-CA-C	5.92	117.92	110.70
23	LU	54	GLY	CA-C-N	5.92	132.84	121.54
23	LU	54	GLY	C-N-CA	5.92	132.84	121.54
70	SM	125	GLU	N-CA-CB	5.90	120.02	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	LP	131	ARG	Peptide

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Mol	Chain	Res	Type	Group
56	SQ	145	TYR	Peptide
56	SQ	43	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	80211	0	40469	456	0
2	L2	2558	0	1296	12	0
3	L3	3316	0	1687	16	0
4	LA	1898	0	1993	27	0
5	LB	3238	0	3376	28	0
6	LC	2908	0	3082	16	0
7	LD	2382	0	2410	13	0
8	LE	1765	0	1917	20	0
9	LF	1870	0	1996	15	0
10	LG	1835	0	1976	26	0
11	LH	1518	0	1601	17	0
12	LI	1639	0	1687	19	0
13	LJ	1353	0	1393	12	0
14	LL	1701	0	1818	13	0
15	LM	1138	0	1204	7	0
16	LN	1701	0	1749	20	0
17	LO	1650	0	1794	14	0
18	LP	1242	0	1269	10	0
19	LQ	1513	0	1628	13	0
20	LR	1566	0	1729	12	0
21	LS	1461	0	1502	12	0
22	LT	1298	0	1366	13	0
23	LU	825	0	850	13	0
24	LV	979	0	1039	6	0
25	LW	1015	0	1079	10	0
26	LX	967	0	1040	1	0
27	LY	1115	0	1205	15	0
28	LZ	1106	0	1182	8	0
28	La	1162	0	1213	15	0
29	Lb	876	0	948	10	0
30	Lc	764	0	804	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Ld	888	0	930	3	0
32	Le	1053	0	1147	12	0
33	Lf	876	0	912	6	0
34	Lg	906	0	998	9	0
35	Lh	1015	0	1148	12	0
36	Li	832	0	917	2	0
37	Lj	705	0	737	8	0
38	Lk	569	0	637	4	0
39	Ll	444	0	483	4	0
40	Lm	429	0	465	8	0
41	Ln	230	0	276	2	0
42	Lo	843	0	912	6	0
43	Lp	708	0	756	9	0
44	Lr	1002	0	1068	5	0
45	S2	36959	0	18651	292	0
46	SA	1747	0	1751	22	0
47	SB	1738	0	1809	27	0
48	SD	1765	0	1865	20	0
49	SE	2076	0	2177	30	0
50	SF	1461	0	1511	21	0
51	SH	1497	0	1590	23	0
52	SI	1686	0	1772	21	0
53	SK	827	0	854	15	0
54	SL	1182	0	1253	9	0
55	SP	1045	0	1095	19	0
56	SQ	1142	0	1213	22	0
57	SR	1090	0	1149	9	0
58	SS	1198	0	1261	25	0
59	ST	1112	0	1146	12	0
60	SU	821	0	883	10	0
61	SV	636	0	637	6	0
62	SX	1098	0	1167	10	0
63	Sa	821	0	870	6	0
64	Sc	506	0	536	8	0
65	Sd	459	0	448	8	0
66	Sg	2436	0	2393	42	0
67	SC	1725	0	1813	19	0
68	SG	1923	0	2089	36	0
69	SJ	1525	0	1640	28	0
70	SM	940	0	965	19	0
71	SN	1208	0	1294	7	0
72	SO	1010	0	1034	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	SW	1034	0	1080	9	0
74	SY	1022	0	1088	17	0
75	SZ	598	0	656	5	0
76	Sb	651	0	670	8	0
77	Se	459	0	503	8	0
78	CE	603	0	660	9	0
78	Sf	497	0	495	7	0
79	CC	1589	0	810	34	0
80	CC	1	0	0	0	0
80	L1	264	0	0	0	0
80	L2	3	0	0	0	0
80	L3	5	0	0	0	0
80	LA	1	0	0	0	0
80	LC	2	0	0	0	0
80	LI	1	0	0	0	0
80	LN	1	0	0	0	0
80	LP	1	0	0	0	0
80	LV	1	0	0	0	0
80	Le	1	0	0	0	0
80	Lf	1	0	0	0	0
80	Lg	1	0	0	0	0
80	S2	135	0	0	0	0
80	SG	1	0	0	0	0
80	SJ	1	0	0	0	0
80	Sd	1	0	0	0	0
81	L1	12	0	0	0	0
82	Lg	1	0	0	0	0
82	Lj	1	0	0	0	0
82	Lm	1	0	0	0	0
82	Lo	1	0	0	0	0
82	Lp	1	0	0	0	0
82	Sa	1	0	0	0	0
82	Sb	1	0	0	0	0
82	Sd	1	0	0	0	0
82	Sf	1	0	0	0	0
83	CE	1	0	0	0	0
83	L1	762	0	0	5	0
83	L2	3	0	0	0	0
83	L3	6	0	0	0	0
83	LA	6	0	0	0	0
83	LB	3	0	0	0	0
83	LC	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	LD	1	0	0	0	0
83	LI	2	0	0	0	0
83	LL	1	0	0	0	0
83	LN	1	0	0	0	0
83	LP	1	0	0	0	0
83	LR	1	0	0	0	0
83	LX	2	0	0	0	0
83	LY	2	0	0	1	0
83	La	8	0	0	0	0
83	Lb	1	0	0	0	0
83	Le	2	0	0	0	0
83	Lg	2	0	0	0	0
83	Lj	4	0	0	0	0
83	Ll	2	0	0	0	0
83	Lo	1	0	0	0	0
83	S2	10	0	0	0	0
83	SX	1	0	0	0	0
All	All	218434	0	160516	1570	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1570 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S2:814:5MU:C4	45:S2:814:5MU:C5	1.79	1.63
1:L1:3762:B8H:C6	1:L1:3762:B8H:N1	1.67	1.52
1:L1:3762:B8H:C4	1:L1:3762:B8H:C5	1.84	1.50
1:L1:1:C:N4	3:L3:156:U:H3	1.46	1.12
45:S2:628:A:N6	45:S2:1500:G:H21	1.47	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	230 (94%)	16 (6%)	0	100	100
5	LB	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
6	LC	363/427 (85%)	354 (98%)	9 (2%)	0	100	100
7	LD	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
8	LE	214/288 (74%)	205 (96%)	9 (4%)	0	100	100
9	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
10	LG	223/266 (84%)	218 (98%)	5 (2%)	0	100	100
11	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
12	LI	198/214 (92%)	190 (96%)	8 (4%)	0	100	100
13	LJ	167/178 (94%)	161 (96%)	6 (4%)	0	100	100
14	LL	208/211 (99%)	196 (94%)	12 (6%)	0	100	100
15	LM	137/215 (64%)	132 (96%)	5 (4%)	0	100	100
16	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	LO	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
20	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
21	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
22	LT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
23	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
24	LV	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
25	LW	122/157 (78%)	118 (97%)	4 (3%)	0	100	100
26	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
27	LY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
28	LZ	133/282 (47%)	126 (95%)	7 (5%)	0	100	100
28	La	145/282 (51%)	139 (96%)	6 (4%)	0	100	100
29	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
30	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
31	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
32	Le	126/135 (93%)	119 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
34	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
35	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
36	Li	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
37	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
38	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
39	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
40	Lm	50/128 (39%)	50 (100%)	0	0	100	100
41	Ln	22/25 (88%)	22 (100%)	0	0	100	100
42	Lo	100/106 (94%)	97 (97%)	3 (3%)	0	100	100
43	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
44	Lr	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
46	SA	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
47	SB	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
48	SD	225/243 (93%)	220 (98%)	5 (2%)	0	100	100
49	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
50	SF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
51	SH	182/194 (94%)	169 (93%)	11 (6%)	2 (1%)	11	29
52	SI	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
53	SK	96/165 (58%)	90 (94%)	5 (5%)	1 (1%)	12	32
54	SL	140/158 (89%)	131 (94%)	9 (6%)	0	100	100
55	SP	125/145 (86%)	120 (96%)	5 (4%)	0	100	100
56	SQ	142/146 (97%)	128 (90%)	14 (10%)	0	100	100
57	SR	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
58	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
59	ST	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
60	SU	102/119 (86%)	95 (93%)	6 (6%)	1 (1%)	12	32
61	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
62	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
63	Sa	100/115 (87%)	94 (94%)	5 (5%)	1 (1%)	12	32
64	Sc	62/69 (90%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
66	Sg	311/317 (98%)	292 (94%)	18 (6%)	1 (0%)	36	60
67	SC	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
68	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
69	SJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	24	48
70	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
71	SN	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
72	SO	133/151 (88%)	126 (95%)	6 (4%)	1 (1%)	16	37
73	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
74	SY	123/133 (92%)	117 (95%)	6 (5%)	0	100	100
75	SZ	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
76	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
77	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
78	CE	70/133 (53%)	67 (96%)	3 (4%)	0	100	100
78	Sf	59/133 (44%)	52 (88%)	7 (12%)	0	100	100
All	All	11319/13078 (86%)	10904 (96%)	407 (4%)	8 (0%)	49	73

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	SU	94	PRO
51	SH	34	SER
51	SH	35	ASP
66	Sg	50	THR
69	SJ	122	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	189 (100%)	1 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LB	348/349 (100%)	347 (100%)	1 (0%)	86	94
6	LC	304/348 (87%)	303 (100%)	1 (0%)	86	94
7	LD	246/250 (98%)	246 (100%)	0	100	100
8	LE	194/252 (77%)	194 (100%)	0	100	100
9	LF	194/215 (90%)	192 (99%)	2 (1%)	68	86
10	LG	196/223 (88%)	196 (100%)	0	100	100
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	172/181 (95%)	170 (99%)	2 (1%)	63	84
13	LJ	142/149 (95%)	142 (100%)	0	100	100
14	LL	176/177 (99%)	176 (100%)	0	100	100
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	170 (99%)	1 (1%)	78	91
17	LO	173/174 (99%)	173 (100%)	0	100	100
18	LP	134/163 (82%)	134 (100%)	0	100	100
19	LQ	164/165 (99%)	164 (100%)	0	100	100
20	LR	166/175 (95%)	163 (98%)	3 (2%)	51	78
21	LS	157/157 (100%)	157 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	91 (100%)	0	100	100
24	LV	101/107 (94%)	101 (100%)	0	100	100
25	LW	103/126 (82%)	103 (100%)	0	100	100
26	LX	106/133 (80%)	106 (100%)	0	100	100
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/237 (49%)	117 (100%)	0	100	100
28	La	120/237 (51%)	120 (100%)	0	100	100
29	Lb	88/126 (70%)	88 (100%)	0	100	100
30	Lc	83/97 (86%)	83 (100%)	0	100	100
31	Ld	98/110 (89%)	98 (100%)	0	100	100
32	Le	114/121 (94%)	114 (100%)	0	100	100
33	Lf	88/89 (99%)	88 (100%)	0	100	100
34	Lg	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Lh	109/110 (99%)	109 (100%)	0	100	100
36	Li	86/89 (97%)	86 (100%)	0	100	100
37	Lj	73/80 (91%)	73 (100%)	0	100	100
38	Lk	64/65 (98%)	64 (100%)	0	100	100
39	Ll	47/48 (98%)	47 (100%)	0	100	100
40	Lm	48/116 (41%)	48 (100%)	0	100	100
41	Ln	23/24 (96%)	23 (100%)	0	100	100
42	Lo	90/93 (97%)	90 (100%)	0	100	100
43	Lp	74/75 (99%)	74 (100%)	0	100	100
44	Lr	109/121 (90%)	109 (100%)	0	100	100
46	SA	184/243 (76%)	184 (100%)	0	100	100
47	SB	195/231 (84%)	195 (100%)	0	100	100
48	SD	190/202 (94%)	190 (100%)	0	100	100
49	SE	224/225 (100%)	224 (100%)	0	100	100
50	SF	156/170 (92%)	156 (100%)	0	100	100
51	SH	166/174 (95%)	165 (99%)	1 (1%)	78	91
52	SI	178/180 (99%)	178 (100%)	0	100	100
53	SK	89/136 (65%)	89 (100%)	0	100	100
54	SL	130/142 (92%)	130 (100%)	0	100	100
55	SP	113/130 (87%)	113 (100%)	0	100	100
56	SQ	119/121 (98%)	119 (100%)	0	100	100
57	SR	122/122 (100%)	122 (100%)	0	100	100
58	SS	126/132 (96%)	126 (100%)	0	100	100
59	ST	113/115 (98%)	113 (100%)	0	100	100
60	SU	94/107 (88%)	93 (99%)	1 (1%)	65	85
61	SV	67/67 (100%)	62 (92%)	5 (8%)	12	31
62	SX	113/115 (98%)	113 (100%)	0	100	100
63	Sa	89/98 (91%)	89 (100%)	0	100	100
64	Sc	57/62 (92%)	57 (100%)	0	100	100
65	Sd	48/49 (98%)	48 (100%)	0	100	100
66	Sg	272/275 (99%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	SC	188/225 (84%)	188 (100%)	0	100	100
68	SG	207/218 (95%)	203 (98%)	4 (2%)	50	77
69	SJ	161/168 (96%)	161 (100%)	0	100	100
70	SM	102/108 (94%)	102 (100%)	0	100	100
71	SN	130/131 (99%)	130 (100%)	0	100	100
72	SO	105/119 (88%)	105 (100%)	0	100	100
73	SW	112/113 (99%)	112 (100%)	0	100	100
74	SY	109/115 (95%)	109 (100%)	0	100	100
75	SZ	66/103 (64%)	66 (100%)	0	100	100
76	Sb	75/76 (99%)	75 (100%)	0	100	100
77	Se	47/48 (98%)	47 (100%)	0	100	100
78	CE	68/122 (56%)	68 (100%)	0	100	100
78	Sf	54/122 (44%)	54 (100%)	0	100	100
All	All	9876/11139 (89%)	9854 (100%)	22 (0%)	85	95

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
61	SV	80	SER
61	SV	83	PHE
61	SV	82	ASN
68	SG	215	LYS
12	LI	15	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
53	SK	42	ASN
59	ST	142	ASN
53	SK	84	HIS
56	SQ	86	GLN
66	Sg	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3705/5070 (73%)	746 (20%)	12 (0%)
2	L2	119/121 (98%)	11 (9%)	0
3	L3	155/157 (98%)	34 (21%)	0
45	S2	1715/1869 (91%)	335 (19%)	9 (0%)
79	CC	74/75 (98%)	23 (31%)	2 (2%)
All	All	5768/7292 (79%)	1149 (19%)	23 (0%)

5 of 1149 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	39	A
1	L1	48	G
1	L1	56	A
1	L1	59	A
1	L1	64	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	S2	628	A
45	S2	954	U
45	S2	867	OMG
45	S2	1434	C
1	L1	1633	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

144 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMG	L1	4196	1	23,26,27	2.36	9 (39%)	33,38,41	1.96	10 (30%)
45	OMU	S2	1442	45,80	19,22,23	2.94	7 (36%)	26,31,34	1.66	4 (15%)
1	OMU	L1	4498	1	19,22,23	2.85	7 (36%)	26,31,34	1.78	4 (15%)
45	OMC	S2	1391	45	19,22,23	3.02	8 (42%)	26,31,34	0.85	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	L1	4335	1	18,22,23	3.51	7 (38%)	26,32,35	0.99	2 (7%)
45	OMU	S2	116	45	19,22,23	2.83	6 (31%)	26,31,34	1.71	5 (19%)
1	OMC	L1	3869	1	19,22,23	2.94	8 (42%)	26,31,34	0.74	0
45	OMU	S2	354	45	19,22,23	2.89	7 (36%)	26,31,34	1.80	5 (19%)
1	A2M	L1	3867	1	22,25,26	3.37	9 (40%)	31,36,39	2.73	10 (32%)
45	OMG	S2	436	45	23,26,27	2.42	8 (34%)	33,38,41	2.04	10 (30%)
45	OMG	S2	683	45	23,26,27	2.42	8 (34%)	33,38,41	2.09	10 (30%)
45	5MC	S2	1374	45	18,22,23	3.53	7 (38%)	26,32,35	1.02	2 (7%)
1	A2M	L1	1326	1	22,25,26	3.34	8 (36%)	31,36,39	2.58	9 (29%)
1	6MZ	L1	4220	1	22,25,26	2.64	3 (13%)	30,36,39	2.20	8 (26%)
1	OMC	L1	3808	1,80	19,22,23	2.94	8 (42%)	26,31,34	1.04	1 (3%)
1	PSU	L1	4450	1,80	18,21,22	1.11	1 (5%)	22,30,33	1.83	3 (13%)
45	A2M	S2	99	45,80	22,25,26	3.43	10 (45%)	31,36,39	2.59	9 (29%)
1	A2M	L1	2787	1	22,25,26	3.45	8 (36%)	31,36,39	2.63	9 (29%)
1	OMC	L1	4536	1	19,22,23	2.91	8 (42%)	26,31,34	0.75	0
1	OMG	L1	1522	1	23,26,27	2.42	9 (39%)	33,38,41	2.09	12 (36%)
1	OMC	L1	2824	1	19,22,23	2.93	8 (42%)	26,31,34	0.99	2 (7%)
1	OMG	L1	3627	1	23,26,27	2.42	8 (34%)	33,38,41	2.08	10 (30%)
1	OMG	L1	1625	1	23,26,27	1.32	3 (13%)	33,38,41	1.93	6 (18%)
45	PSU	S2	1081	45	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
1	A2M	L1	400	1	22,25,26	3.43	9 (40%)	31,36,39	2.66	8 (25%)
1	A2M	L1	398	1	22,25,26	3.44	9 (40%)	31,36,39	2.69	11 (35%)
1	OMG	L1	4637	1	23,26,27	2.37	7 (30%)	33,38,41	2.02	10 (30%)
1	OMG	L1	4618	1	23,26,27	2.40	7 (30%)	33,38,41	2.06	10 (30%)
45	A2M	S2	27	45,80	22,25,26	3.43	9 (40%)	31,36,39	2.68	9 (29%)
1	A2M	L1	1534	1,80	22,25,26	3.47	10 (45%)	31,36,39	2.65	8 (25%)
1	PSU	L1	1582	1	18,21,22	1.07	1 (5%)	22,30,33	1.57	4 (18%)
1	OMG	L1	3944	1	23,26,27	2.45	8 (34%)	33,38,41	2.02	10 (30%)
1	OMU	L1	4227	1	19,22,23	2.82	7 (36%)	26,31,34	1.72	4 (15%)
1	OMC	L1	1881	1,80	19,22,23	2.93	8 (42%)	26,31,34	0.95	0
1	OMC	L1	2861	1	19,22,23	2.93	8 (42%)	26,31,34	0.72	0
1	UR3	L1	4530	1	19,22,23	2.75	8 (42%)	26,32,35	1.44	3 (11%)
45	PSU	S2	119	45	18,21,22	0.97	1 (5%)	22,30,33	1.63	4 (18%)
1	OMG	L1	2424	1	23,26,27	2.41	9 (39%)	33,38,41	1.99	10 (30%)
1	OMG	L1	3899	1,80	23,26,27	2.41	9 (39%)	33,38,41	2.10	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMC	S2	1272	45	19,22,23	3.06	8 (42%)	26,31,34	0.81	0
45	OMG	S2	1447	45	23,26,27	1.23	3 (13%)	33,38,41	2.17	9 (27%)
1	A2M	L1	3830	1	22,25,26	3.39	9 (40%)	31,36,39	2.78	10 (32%)
1	UY1	L1	3818	1,80,81	19,22,23	4.44	12 (63%)	22,31,34	2.02	4 (18%)
1	PSU	L1	4531	1	18,21,22	1.00	1 (5%)	22,30,33	1.70	4 (18%)
45	OMC	S2	1703	45	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
1	OMG	L1	4623	1	23,26,27	2.38	9 (39%)	33,38,41	2.08	10 (30%)
45	OMU	S2	172	45	19,22,23	2.88	6 (31%)	26,31,34	1.76	5 (19%)
1	OMG	L1	4494	1	23,26,27	2.36	8 (34%)	33,38,41	2.04	9 (27%)
45	6MZ	S2	1832	45,80	22,25,26	2.88	4 (18%)	30,36,39	2.24	10 (33%)
45	M7A	S2	1806	45	20,25,26	1.86	5 (25%)	28,37,40	3.94	8 (28%)
1	2MG	L1	729	1	23,26,27	2.60	9 (39%)	32,38,41	2.30	11 (34%)
45	PSU	S2	612	45	18,21,22	1.02	1 (5%)	22,30,33	1.81	5 (22%)
3	OMU	L3	14	3,1	19,22,23	2.88	6 (31%)	26,31,34	1.71	5 (19%)
45	4AC	S2	1842	45	21,24,25	3.40	10 (47%)	29,34,37	1.09	2 (6%)
45	OMG	S2	509	45,80	23,26,27	2.36	8 (34%)	33,38,41	1.95	9 (27%)
45	A2M	S2	484	45	22,25,26	3.40	9 (40%)	31,36,39	2.63	10 (32%)
1	A2M	L1	2363	1,80	22,25,26	3.46	9 (40%)	31,36,39	2.70	8 (25%)
1	PSU	L1	4403	1	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
45	A2M	S2	1383	45	22,25,26	3.38	8 (36%)	31,36,39	2.73	8 (25%)
1	PSU	L1	3729	1	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
45	OMC	S2	1710	45	19,22,23	3.04	8 (42%)	26,31,34	0.83	1 (3%)
45	JMH	S2	1219	45,80	18,22,23	2.84	5 (27%)	21,32,35	1.74	4 (19%)
1	B8T	L1	4671	1	19,22,23	3.21	8 (42%)	26,31,34	0.98	1 (3%)
1	OMG	L1	2876	1	23,26,27	2.42	8 (34%)	33,38,41	2.12	8 (24%)
3	OMG	L3	75	3	23,26,27	2.42	8 (34%)	33,38,41	2.03	10 (30%)
1	A2M	L1	4523	1,80	22,25,26	3.37	9 (40%)	31,36,39	2.61	9 (29%)
45	5MU	S2	814	45	19,22,23	7.26	8 (42%)	28,32,35	3.30	12 (42%)
1	B8H	L1	3762	1	19,22,23	6.72	6 (31%)	22,32,35	2.39	5 (22%)
45	OMG	S2	601	45	23,26,27	2.39	8 (34%)	33,38,41	2.02	10 (30%)
1	OMG	L1	1316	1,80	23,26,27	2.41	7 (30%)	33,38,41	2.04	10 (30%)
45	OMG	S2	867	45	23,26,27	2.43	8 (34%)	33,38,41	2.01	9 (27%)
1	PSU	L1	3764	1	18,21,22	1.02	1 (5%)	22,30,33	1.65	4 (18%)
1	A2M	L1	3718	1	22,25,26	3.42	9 (40%)	31,36,39	2.51	10 (32%)
1	JMH	L1	1456	1	18,22,23	2.64	5 (27%)	21,32,35	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A2M	S2	468	45	22,25,26	3.41	10 (45%)	31,36,39	2.69	10 (32%)
45	A2M	S2	166	45	22,25,26	3.42	9 (40%)	31,36,39	2.72	8 (25%)
45	OMC	S2	462	45	19,22,23	2.97	8 (42%)	26,31,34	0.75	0
1	OMG	L1	4228	1	23,26,27	2.39	9 (39%)	33,38,41	2.05	10 (30%)
45	PSU	S2	823	45	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
45	OMU	S2	428	45	19,22,23	2.92	7 (36%)	26,31,34	1.71	4 (15%)
45	A2M	S2	1678	45	22,25,26	3.47	9 (40%)	31,36,39	2.73	11 (35%)
1	PSU	L1	1677	1,81	18,21,22	1.16	2 (11%)	22,30,33	1.94	5 (22%)
45	A2M	S2	159	45	22,25,26	3.43	9 (40%)	31,36,39	2.73	10 (32%)
1	A2M	L1	3723	1	22,25,26	3.43	9 (40%)	31,36,39	2.61	9 (29%)
1	OMU	L1	3925	1	19,22,23	2.85	6 (31%)	26,31,34	1.92	5 (19%)
45	OMU	S2	1288	45	19,22,23	2.94	8 (42%)	26,31,34	1.64	4 (15%)
1	PSU	L1	2508	1	18,21,22	1.04	1 (5%)	22,30,33	1.70	3 (13%)
1	A2M	L1	1524	1	22,25,26	3.41	10 (45%)	31,36,39	2.70	11 (35%)
1	OMC	L1	2365	1,80	19,22,23	2.90	8 (42%)	26,31,34	0.62	0
45	4AC	S2	1337	45	21,24,25	3.51	10 (47%)	29,34,37	1.07	2 (6%)
1	A2M	L1	4571	1	22,25,26	3.45	9 (40%)	31,36,39	2.59	8 (25%)
45	OMG	S2	1490	45,80	23,26,27	2.42	8 (34%)	33,38,41	1.92	9 (27%)
1	A2M	L1	2815	1	22,25,26	3.41	10 (45%)	31,36,39	2.65	8 (25%)
1	A2M	L1	1871	1,80	22,25,26	3.44	10 (45%)	31,36,39	2.72	11 (35%)
1	PSU	L1	4628	1	18,21,22	0.92	1 (5%)	22,30,33	1.69	3 (13%)
45	OMG	S2	1328	45	23,26,27	2.44	8 (34%)	33,38,41	2.01	10 (30%)
45	PSU	S2	1243	45	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
1	2MG	L1	978	1	23,26,27	2.65	9 (39%)	32,38,41	2.32	12 (37%)
1	OMU	L1	2837	1	19,22,23	2.84	6 (31%)	26,31,34	1.73	5 (19%)
45	OMG	S2	644	45	23,26,27	2.41	8 (34%)	33,38,41	2.00	10 (30%)
45	UY1	S2	1326	45,80	19,22,23	4.33	10 (52%)	22,31,34	1.84	3 (13%)
1	OMC	L1	3841	1	19,22,23	2.94	8 (42%)	26,31,34	0.91	1 (3%)
1	OMC	L1	3701	1,80	19,22,23	2.88	8 (42%)	26,31,34	0.84	0
1	OMU	L1	4306	1	19,22,23	2.79	6 (31%)	26,31,34	1.66	4 (15%)
1	5MC	L1	4447	1,80	18,22,23	3.41	7 (38%)	26,32,35	1.15	2 (7%)
42	MLZ	Lo	53	42	8,9,10	0.68	0	4,9,11	0.58	0
45	PSU	S2	822	45	18,21,22	1.05	1 (5%)	22,30,33	1.77	5 (22%)
45	A2M	S2	1031	45	22,25,26	3.38	10 (45%)	31,36,39	2.63	9 (29%)
1	OMG	L1	4499	1	23,26,27	2.41	8 (34%)	33,38,41	2.06	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	MA6	S2	1851	45	23,26,27	1.31	4 (17%)	34,38,41	4.59	12 (35%)
1	OMG	L1	3792	1	23,26,27	2.40	8 (34%)	33,38,41	2.00	10 (30%)
1	A2M	L1	3825	1	22,25,26	3.41	9 (40%)	31,36,39	2.68	8 (25%)
1	PSU	L1	4636	1	18,21,22	1.09	1 (5%)	22,30,33	1.93	5 (22%)
1	OMG	L1	4370	1	23,26,27	2.37	8 (34%)	33,38,41	1.98	9 (27%)
1	OMU	L1	4620	1	19,22,23	2.80	7 (36%)	26,31,34	1.65	4 (15%)
1	OMC	L1	2804	1	19,22,23	2.89	7 (36%)	26,31,34	0.90	0
45	OMC	S2	174	45,80	19,22,23	3.01	8 (42%)	26,31,34	0.75	0
1	A2M	L1	2401	1	22,25,26	3.38	10 (45%)	31,36,39	2.69	9 (29%)
45	A2M	S2	590	45	22,25,26	3.39	9 (40%)	31,36,39	2.82	9 (29%)
1	1MA	L1	1322	1,80	21,25,26	2.66	6 (28%)	31,37,40	2.24	7 (22%)
1	PSU	L1	4500	1	18,21,22	0.98	1 (5%)	22,30,33	1.76	4 (18%)
45	OMU	S2	121	45	19,22,23	2.84	6 (31%)	26,31,34	1.58	4 (15%)
1	OMC	L1	2422	1,80	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
1	PSU	L1	3715	1	18,21,22	1.10	1 (5%)	22,30,33	1.84	5 (22%)
1	A2M	L1	3785	1	22,25,26	3.31	10 (45%)	31,36,39	2.90	10 (32%)
1	OMG	L1	3744	1	23,26,27	2.36	8 (34%)	33,38,41	2.02	10 (30%)
1	OMG	L1	2364	1,80	23,26,27	2.34	9 (39%)	33,38,41	2.06	13 (39%)
1	OMC	L1	4456	1	19,22,23	2.88	8 (42%)	26,31,34	0.86	0
45	A2M	S2	668	45,80	22,25,26	3.42	10 (45%)	31,36,39	2.73	12 (38%)
1	OMC	L1	2351	1	19,22,23	2.87	8 (42%)	26,31,34	1.25	3 (11%)
1	OMC	L1	3887	1	19,22,23	2.92	8 (42%)	26,31,34	0.86	0
45	A2M	S2	576	45	22,25,26	3.40	9 (40%)	31,36,39	2.67	9 (29%)
45	B8N	S2	1248	45	24,29,30	3.11	7 (29%)	29,42,45	1.75	6 (20%)
1	5MC	L1	3782	1,80	18,22,23	3.37	7 (38%)	26,32,35	1.21	3 (11%)
1	2MG	L1	1517	1	23,26,27	2.61	10 (43%)	32,38,41	2.35	12 (37%)
45	A2M	S2	512	45	22,25,26	3.41	9 (40%)	31,36,39	2.75	9 (29%)
45	UR3	S2	1830	45	19,22,23	2.76	7 (36%)	26,32,35	1.61	4 (15%)
1	PSU	L1	1683	1,81	18,21,22	1.10	1 (5%)	22,30,33	1.67	3 (13%)
1	PSU	L1	4442	1	18,21,22	1.09	1 (5%)	22,30,33	1.78	5 (22%)
1	OMC	L1	1340	1	19,22,23	2.89	8 (42%)	26,31,34	0.85	0
45	MA6	S2	1850	45	23,26,27	1.36	4 (17%)	34,38,41	4.17	13 (38%)
1	OMG	L1	4392	1	23,26,27	2.43	7 (30%)	33,38,41	2.03	10 (30%)
1	PSU	L1	4293	1	18,21,22	1.00	1 (5%)	22,30,33	1.68	3 (13%)
45	OMC	S2	517	45	19,22,23	2.98	8 (42%)	26,31,34	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	4196	1	-	1/9/27/28	0/3/3/3
45	OMU	S2	1442	45,80	-	3/9/27/28	0/2/2/2
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
45	OMC	S2	1391	45	-	2/9/27/28	0/2/2/2
1	5MC	L1	4335	1	-	0/7/25/26	0/2/2/2
45	OMU	S2	116	45	-	0/9/27/28	0/2/2/2
1	OMC	L1	3869	1	-	1/9/27/28	0/2/2/2
45	OMU	S2	354	45	-	0/9/27/28	0/2/2/2
1	A2M	L1	3867	1	-	2/9/27/28	0/3/3/3
45	OMG	S2	436	45	-	0/9/27/28	0/3/3/3
45	OMG	S2	683	45	-	2/9/27/28	0/3/3/3
45	5MC	S2	1374	45	-	0/7/25/26	0/2/2/2
1	A2M	L1	1326	1	-	1/9/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	3808	1,80	-	2/9/27/28	0/2/2/2
1	PSU	L1	4450	1,80	-	1/7/25/26	0/2/2/2
45	A2M	S2	99	45,80	-	2/9/27/28	0/3/3/3
1	A2M	L1	2787	1	-	4/9/27/28	0/3/3/3
1	OMC	L1	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	1522	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	2824	1	-	2/9/27/28	0/2/2/2
1	OMG	L1	3627	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	1625	1	-	0/9/27/28	0/3/3/3
45	PSU	S2	1081	45	-	1/7/25/26	0/2/2/2
1	A2M	L1	400	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	398	1	-	2/9/27/28	0/3/3/3
1	OMG	L1	4637	1	-	1/9/27/28	0/3/3/3
1	OMG	L1	4618	1	-	0/9/27/28	0/3/3/3
45	A2M	S2	27	45,80	-	0/9/27/28	0/3/3/3
1	A2M	L1	1534	1,80	-	3/9/27/28	0/3/3/3
1	PSU	L1	1582	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	3944	1	-	2/9/27/28	0/3/3/3
1	OMU	L1	4227	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	1881	1,80	-	0/9/27/28	0/2/2/2
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	S2	119	45	-	0/7/25/26	0/2/2/2
1	OMG	L1	2424	1	-	2/9/27/28	0/3/3/3
1	OMG	L1	3899	1,80	-	0/9/27/28	0/3/3/3
45	OMC	S2	1272	45	-	0/9/27/28	0/2/2/2
45	OMG	S2	1447	45	-	1/9/27/28	0/3/3/3
1	A2M	L1	3830	1	-	0/9/27/28	0/3/3/3
1	UY1	L1	3818	1,80,81	-	4/9/27/28	0/2/2/2
1	PSU	L1	4531	1	-	0/7/25/26	0/2/2/2
45	OMC	S2	1703	45	-	0/9/27/28	0/2/2/2
1	OMG	L1	4623	1	-	0/9/27/28	0/3/3/3
45	OMU	S2	172	45	-	0/9/27/28	0/2/2/2
1	OMG	L1	4494	1	-	0/9/27/28	0/3/3/3
45	6MZ	S2	1832	45,80	-	2/9/27/28	0/3/3/3
45	M7A	S2	1806	45	-	0/7/37/38	0/3/3/3
1	2MG	L1	729	1	-	1/9/27/28	0/3/3/3
45	PSU	S2	612	45	-	0/7/25/26	0/2/2/2
3	OMU	L3	14	3,1	-	1/9/27/28	0/2/2/2
45	4AC	S2	1842	45	-	0/11/29/30	0/2/2/2
45	OMG	S2	509	45,80	-	0/9/27/28	0/3/3/3
45	A2M	S2	484	45	-	0/9/27/28	0/3/3/3
1	A2M	L1	2363	1,80	-	1/9/27/28	0/3/3/3
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	1383	45	-	0/9/27/28	0/3/3/3
1	PSU	L1	3729	1	-	2/7/25/26	0/2/2/2
45	OMC	S2	1710	45	-	0/9/27/28	0/2/2/2
45	JMH	S2	1219	45,80	-	2/7/25/26	0/2/2/2
1	B8T	L1	4671	1	-	1/7/27/28	0/2/2/2
1	OMG	L1	2876	1	-	0/9/27/28	0/3/3/3
3	OMG	L3	75	3	-	0/9/27/28	0/3/3/3
1	A2M	L1	4523	1,80	-	0/9/27/28	0/3/3/3
45	5MU	S2	814	45	-	0/7/25/26	0/2/2/2
1	B8H	L1	3762	1	-	0/7/25/26	0/2/2/2
45	OMG	S2	601	45	-	1/9/27/28	0/3/3/3
1	OMG	L1	1316	1,80	-	0/9/27/28	0/3/3/3
45	OMG	S2	867	45	-	3/9/27/28	0/3/3/3
1	PSU	L1	3764	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	3718	1	-	0/9/27/28	0/3/3/3
1	JMH	L1	1456	1	-	0/7/25/26	0/2/2/2
45	A2M	S2	468	45	-	0/9/27/28	0/3/3/3
45	A2M	S2	166	45	-	0/9/27/28	0/3/3/3
45	OMC	S2	462	45	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	4228	1	-	0/9/27/28	0/3/3/3
45	PSU	S2	823	45	-	0/7/25/26	0/2/2/2
45	OMU	S2	428	45	-	2/9/27/28	0/2/2/2
45	A2M	S2	1678	45	-	1/9/27/28	0/3/3/3
1	PSU	L1	1677	1,81	-	4/7/25/26	0/2/2/2
45	A2M	S2	159	45	-	2/9/27/28	0/3/3/3
1	A2M	L1	3723	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	3925	1	-	1/9/27/28	0/2/2/2
45	OMU	S2	1288	45	-	0/9/27/28	0/2/2/2
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1524	1	-	1/9/27/28	0/3/3/3
1	OMC	L1	2365	1,80	-	0/9/27/28	0/2/2/2
45	4AC	S2	1337	45	-	0/11/29/30	0/2/2/2
1	A2M	L1	4571	1	-	0/9/27/28	0/3/3/3
45	OMG	S2	1490	45,80	-	1/9/27/28	0/3/3/3
1	A2M	L1	2815	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	1871	1,80	-	0/9/27/28	0/3/3/3
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
45	OMG	S2	1328	45	-	1/9/27/28	0/3/3/3
45	PSU	S2	1243	45	-	2/7/25/26	0/2/2/2
1	2MG	L1	978	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
45	OMG	S2	644	45	-	2/9/27/28	0/3/3/3
45	UY1	S2	1326	45,80	-	1/9/27/28	0/2/2/2
1	OMC	L1	3841	1	-	2/9/27/28	0/2/2/2
1	OMC	L1	3701	1,80	-	4/9/27/28	0/2/2/2
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
1	5MC	L1	4447	1,80	-	4/7/25/26	0/2/2/2
42	MLZ	Lo	53	42	-	2/7/8/10	-
45	PSU	S2	822	45	-	1/7/25/26	0/2/2/2
45	A2M	S2	1031	45	-	0/9/27/28	0/3/3/3
1	OMG	L1	4499	1	-	0/9/27/28	0/3/3/3
45	MA6	S2	1851	45	-	2/11/29/30	0/3/3/3
1	OMG	L1	3792	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4636	1	-	3/7/25/26	0/2/2/2
1	OMG	L1	4370	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	4620	1	-	1/9/27/28	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
45	OMC	S2	174	45,80	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	L1	2401	1	-	1/9/27/28	0/3/3/3
45	A2M	S2	590	45	-	4/9/27/28	0/3/3/3
1	1MA	L1	1322	1,80	-	2/7/25/26	0/3/3/3
1	PSU	L1	4500	1	-	3/7/25/26	0/2/2/2
45	OMU	S2	121	45	-	0/9/27/28	0/2/2/2
1	OMC	L1	2422	1,80	-	1/9/27/28	0/2/2/2
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	3785	1	-	2/9/27/28	0/3/3/3
1	OMG	L1	3744	1	-	0/9/27/28	0/3/3/3
1	OMG	L1	2364	1,80	-	2/9/27/28	0/3/3/3
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
45	A2M	S2	668	45,80	-	3/9/27/28	0/3/3/3
1	OMC	L1	2351	1	-	3/9/27/28	0/2/2/2
1	OMC	L1	3887	1	-	0/9/27/28	0/2/2/2
45	A2M	S2	576	45	-	3/9/27/28	0/3/3/3
45	B8N	S2	1248	45	-	3/16/34/35	0/2/2/2
1	5MC	L1	3782	1,80	-	0/7/25/26	0/2/2/2
1	2MG	L1	1517	1	-	0/9/27/28	0/3/3/3
45	A2M	S2	512	45	-	2/9/27/28	0/3/3/3
45	UR3	S2	1830	45	-	2/7/25/26	0/2/2/2
1	PSU	L1	1683	1,81	-	0/7/25/26	0/2/2/2
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1340	1	-	2/9/27/28	0/2/2/2
45	MA6	S2	1850	45	-	3/11/29/30	0/3/3/3
1	OMG	L1	4392	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	4293	1	-	1/7/25/26	0/2/2/2
45	OMC	S2	517	45	-	2/9/27/28	0/2/2/2

The worst 5 of 986 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S2	814	5MU	C4-C5	20.75	1.79	1.44
45	S2	814	5MU	C6-N1	16.52	1.66	1.38
1	L1	3762	B8H	C6-C5	-15.50	1.13	1.34
1	L1	3762	B8H	C4-N3	-14.86	1.11	1.38
1	L1	3762	B8H	C4-C5	14.15	1.84	1.44

The worst 5 of 888 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	S2	1851	MA6	N1-C6-N6	-18.31	97.06	117.08
45	S2	1850	MA6	N1-C6-N6	-15.79	99.82	117.08
45	S2	1806	M7A	C5-C6-N6	13.72	147.18	123.74
45	S2	1806	M7A	N6-C6-N1	-11.74	92.64	118.35
45	S2	1851	MA6	C5-C6-N6	10.50	143.58	125.30

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L1	1340	OMC	C3'-C4'-C5'-O5'
1	L1	1340	OMC	O4'-C4'-C5'-O5'
1	L1	1677	PSU	C2'-C1'-C5-C6
1	L1	2424	OMG	O4'-C4'-C5'-O5'
1	L1	2424	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

48 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	4196	OMG	1	0
1	L1	1326	A2M	1	0
1	L1	4220	6MZ	1	0
1	L1	398	A2M	1	0
1	L1	4637	OMG	1	0
1	L1	4618	OMG	1	0
1	L1	2861	OMC	1	0
45	S2	1447	OMG	1	0
1	L1	3818	UY1	1	0
1	L1	4623	OMG	1	0
45	S2	1832	6MZ	1	0
1	L1	729	2MG	1	0
45	S2	612	PSU	1	0
45	S2	509	OMG	3	0
45	S2	484	A2M	1	0
1	L1	2363	A2M	1	0
3	L3	75	OMG	1	0
45	S2	814	5MU	1	0
1	L1	3762	B8H	6	0
45	S2	601	OMG	1	0
45	S2	867	OMG	1	0
1	L1	3718	A2M	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	1456	JMH	1	0
45	S2	166	A2M	2	0
45	S2	823	PSU	1	0
45	S2	428	OMU	1	0
45	S2	1678	A2M	2	0
1	L1	3723	A2M	1	0
1	L1	3925	OMU	1	0
45	S2	1288	OMU	2	0
45	S2	1490	OMG	2	0
1	L1	1871	A2M	1	0
45	S2	1328	OMG	1	0
45	S2	644	OMG	1	0
1	L1	4447	5MC	1	0
45	S2	1031	A2M	1	0
1	L1	3792	OMG	1	0
1	L1	4370	OMG	2	0
1	L1	2804	OMC	1	0
45	S2	121	OMU	1	0
1	L1	2422	OMC	1	0
1	L1	3744	OMG	1	0
1	L1	2351	OMC	2	0
45	S2	576	A2M	1	0
45	S2	512	A2M	1	0
45	S2	1830	UR3	1	0
1	L1	1340	OMC	1	0
1	L1	4392	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 442 ligands modelled in this entry, 442 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

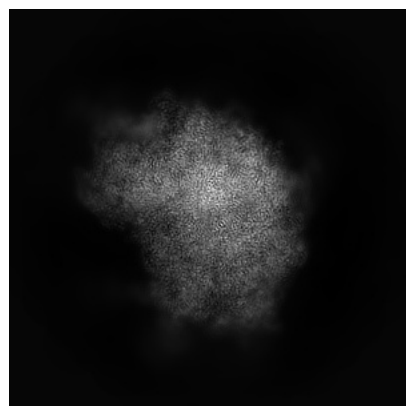
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33329. These allow visual inspection of the internal detail of the map and identification of artifacts.

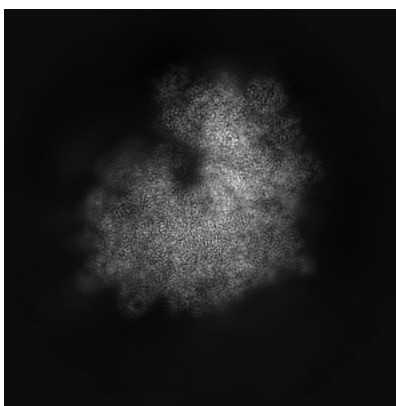
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

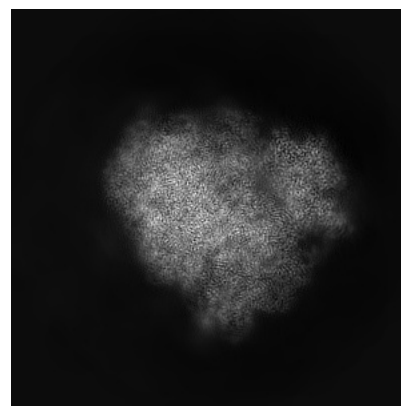
6.1.1 Primary map



X

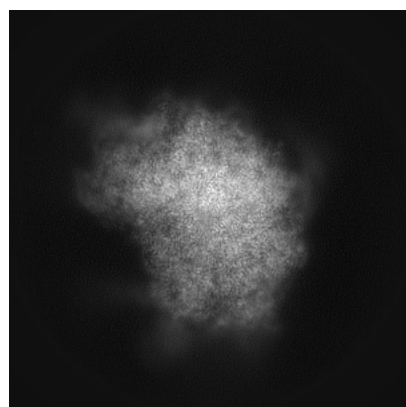


Y

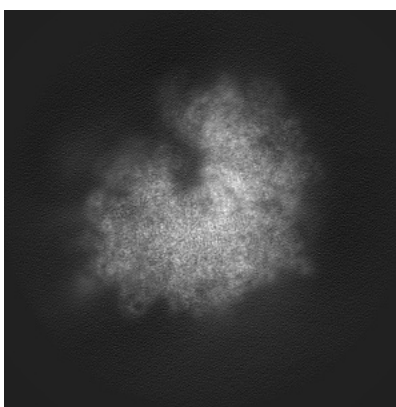


Z

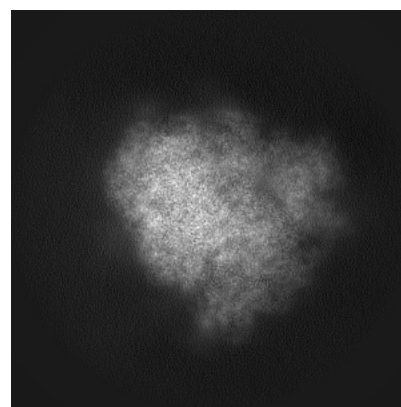
6.1.2 Raw map



X



Y

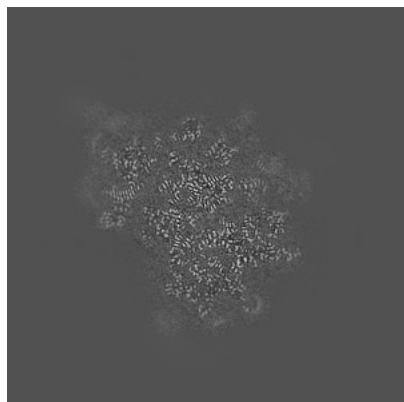


Z

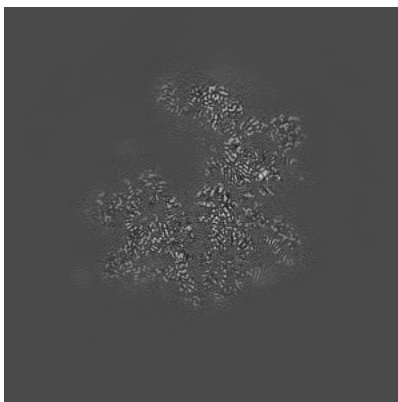
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

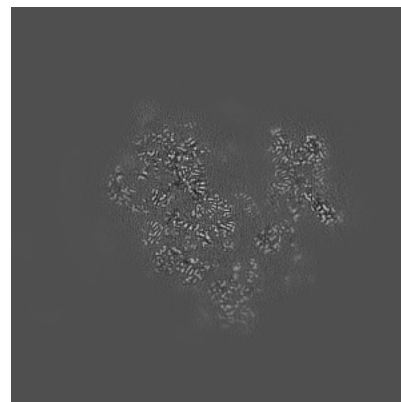
6.2.1 Primary map



X Index: 210

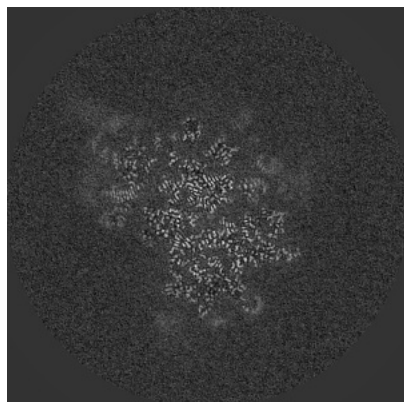


Y Index: 210

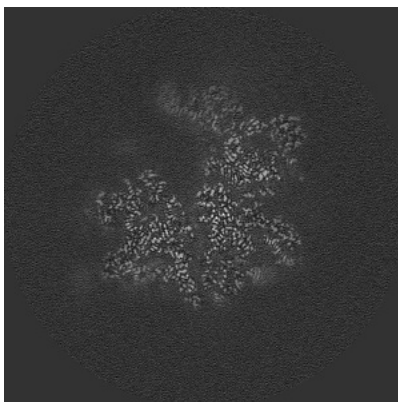


Z Index: 210

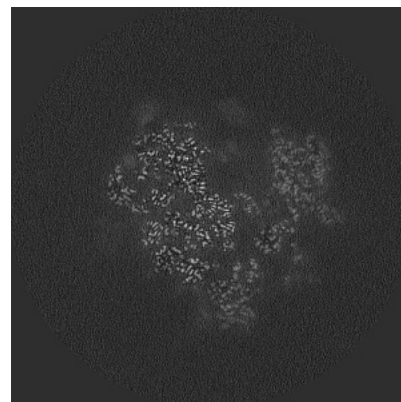
6.2.2 Raw map



X Index: 210



Y Index: 210

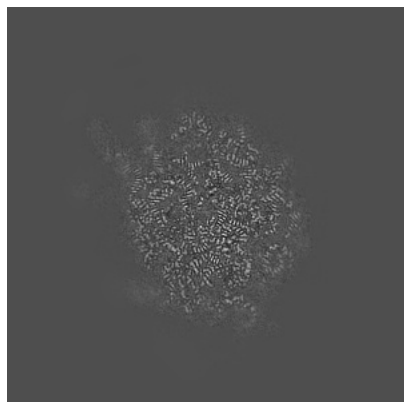


Z Index: 210

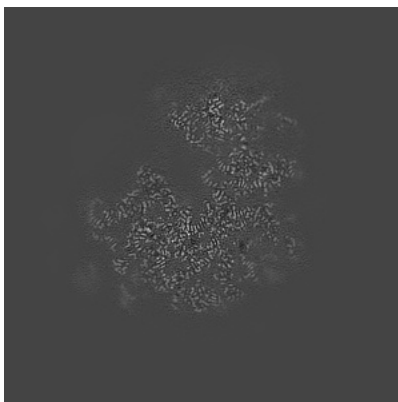
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

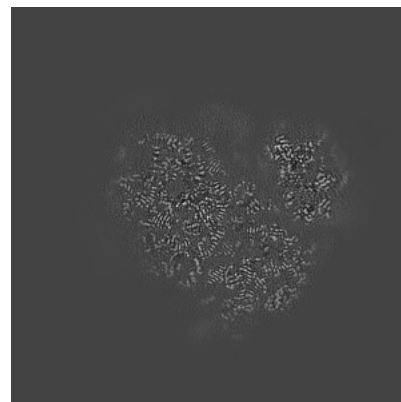
6.3.1 Primary map



X Index: 188

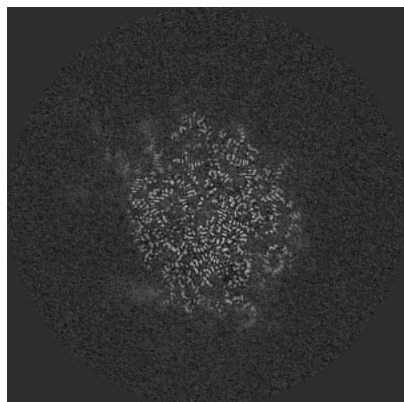


Y Index: 223

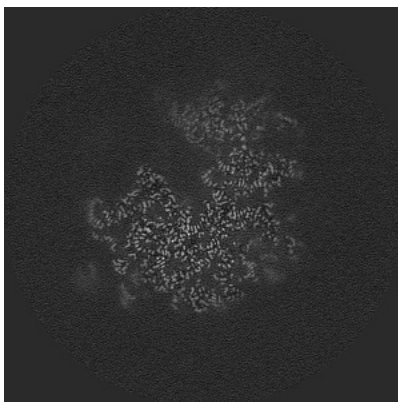


Z Index: 231

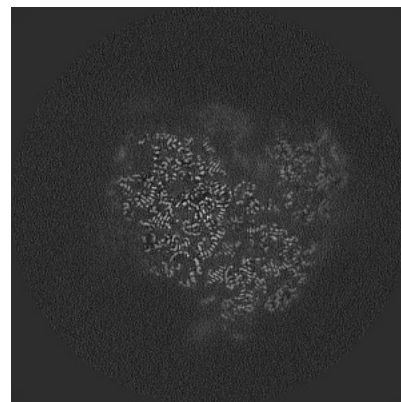
6.3.2 Raw map



X Index: 188



Y Index: 223

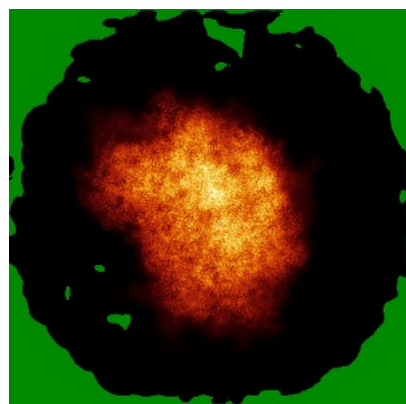


Z Index: 231

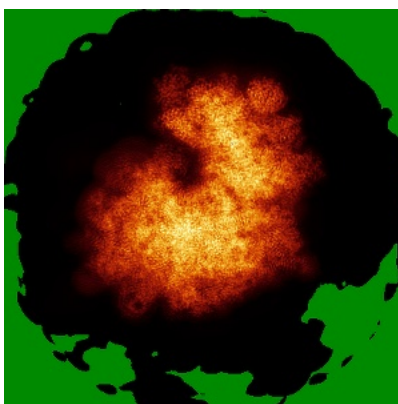
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

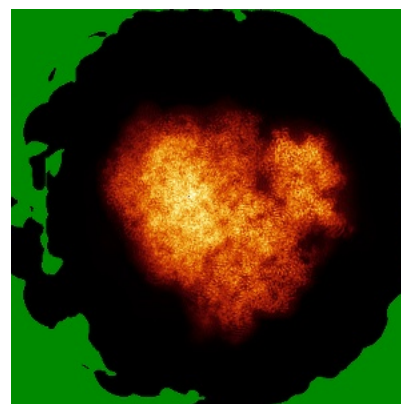
6.4.1 Primary map



X

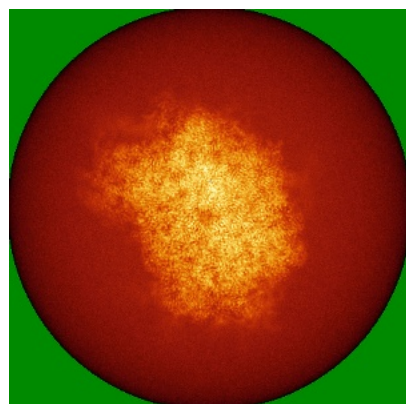


Y

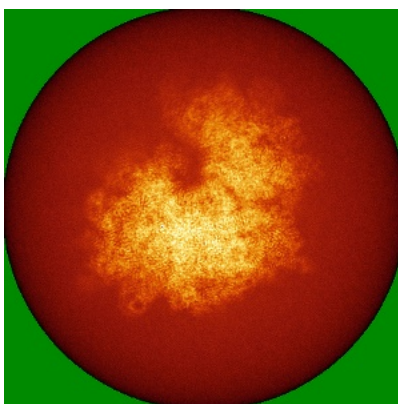


Z

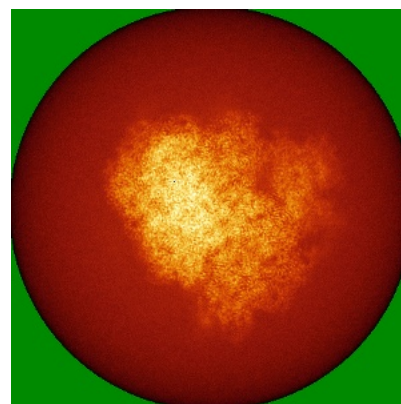
6.4.2 Raw map



X



Y



Z

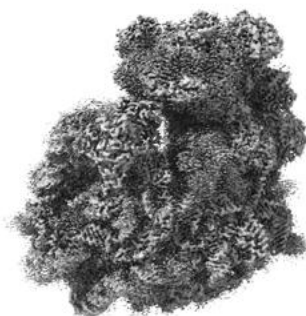
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



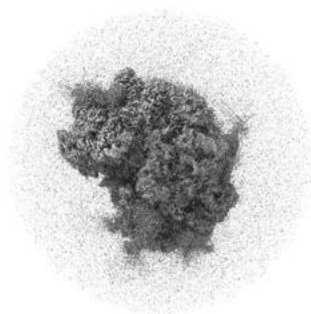
Y



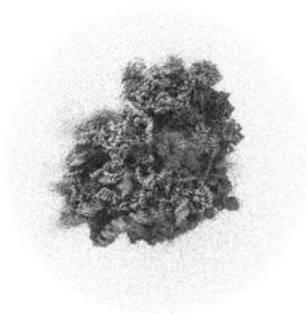
Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

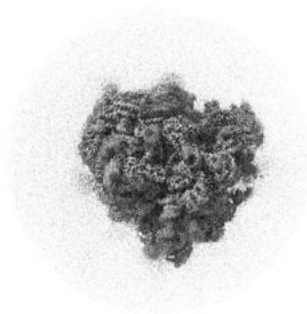
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

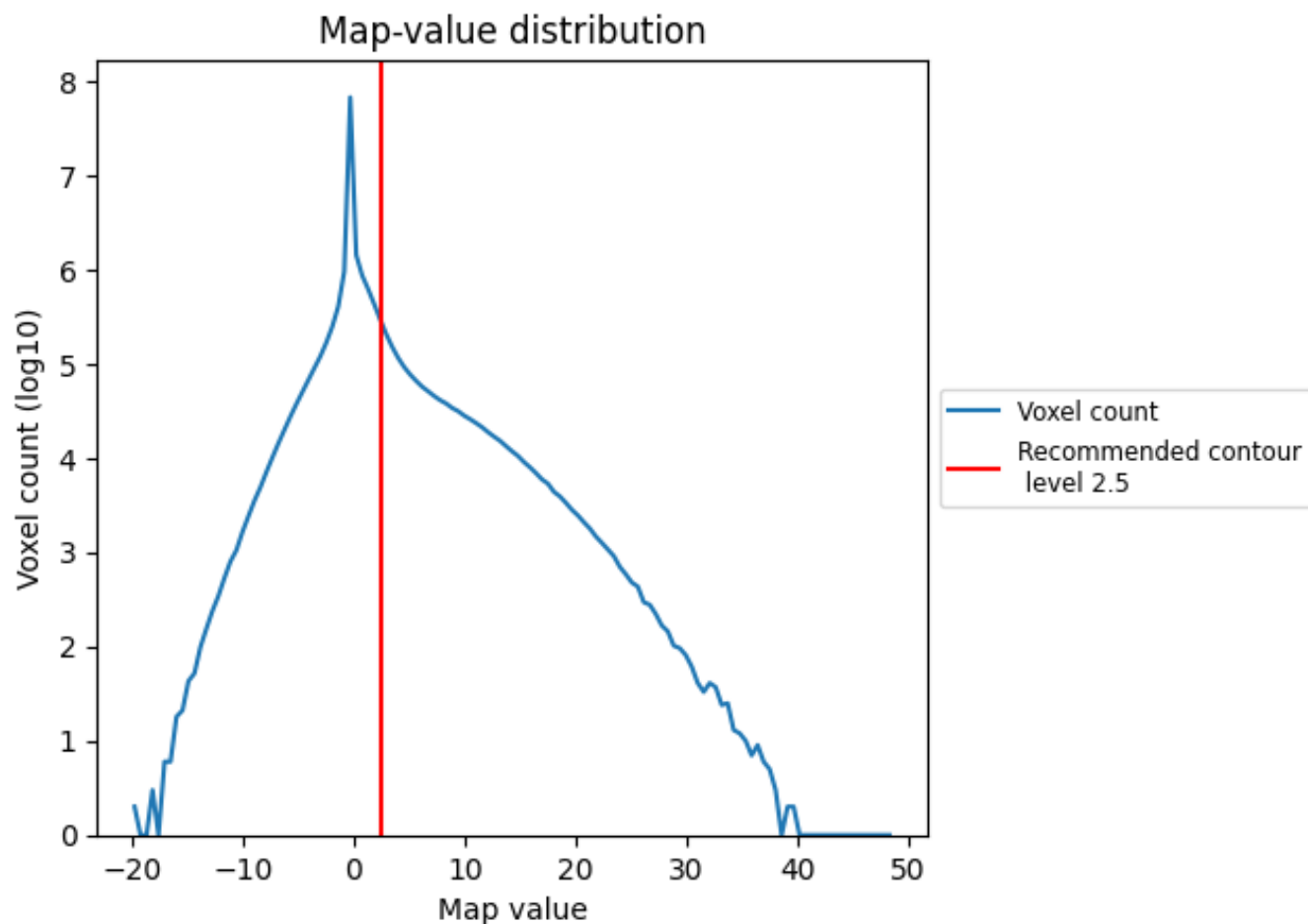
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

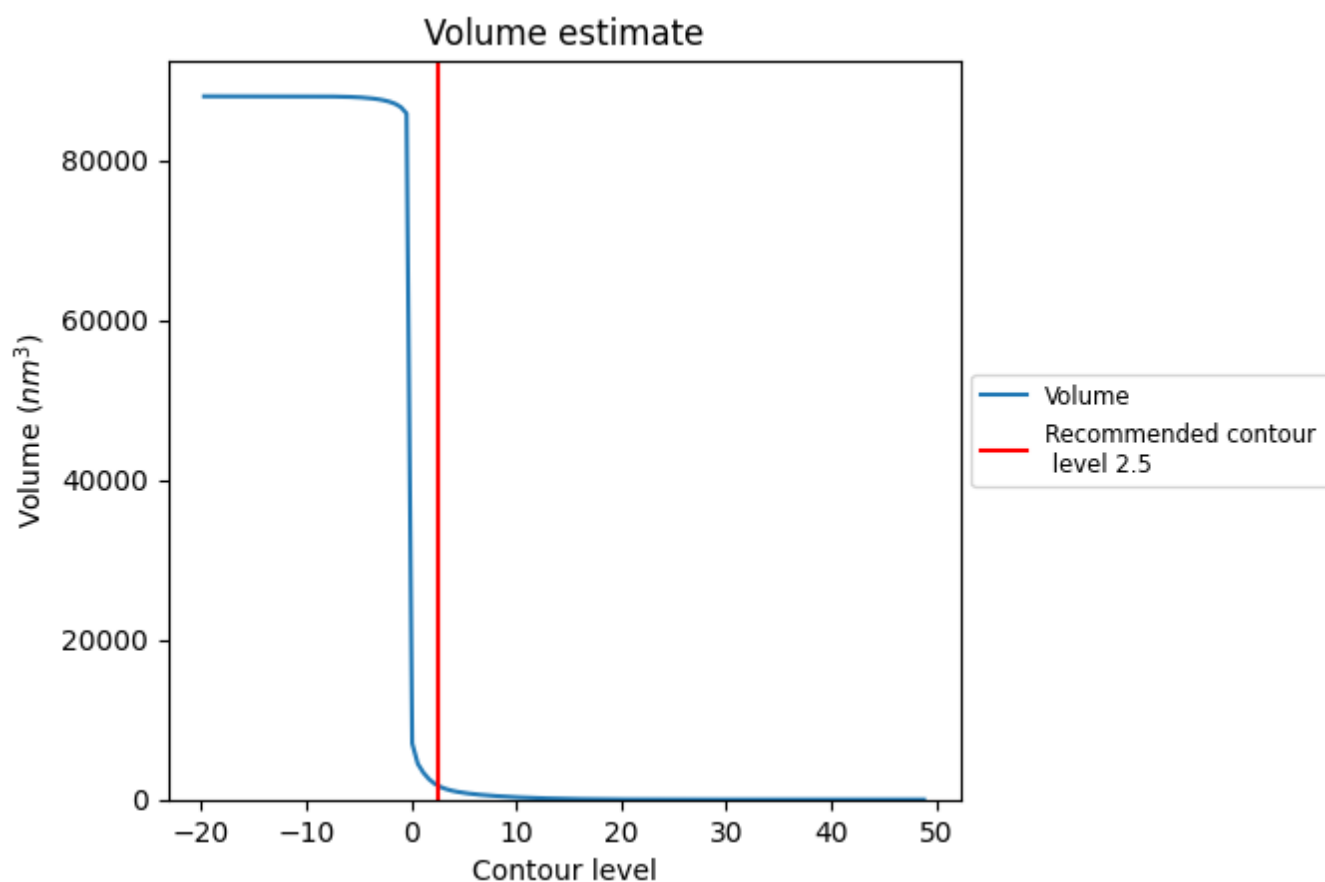
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

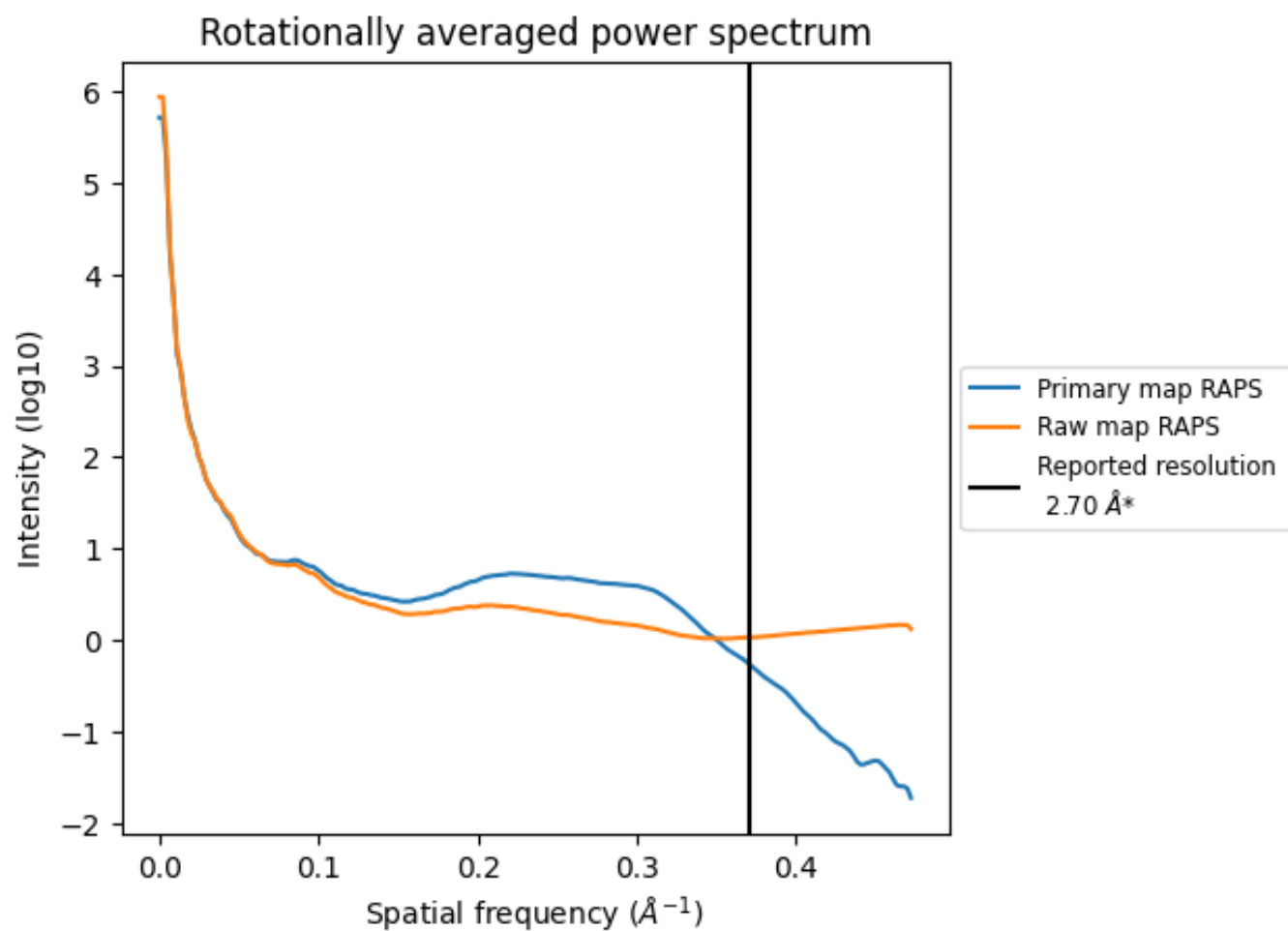
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1791 nm³; this corresponds to an approximate mass of 1617 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

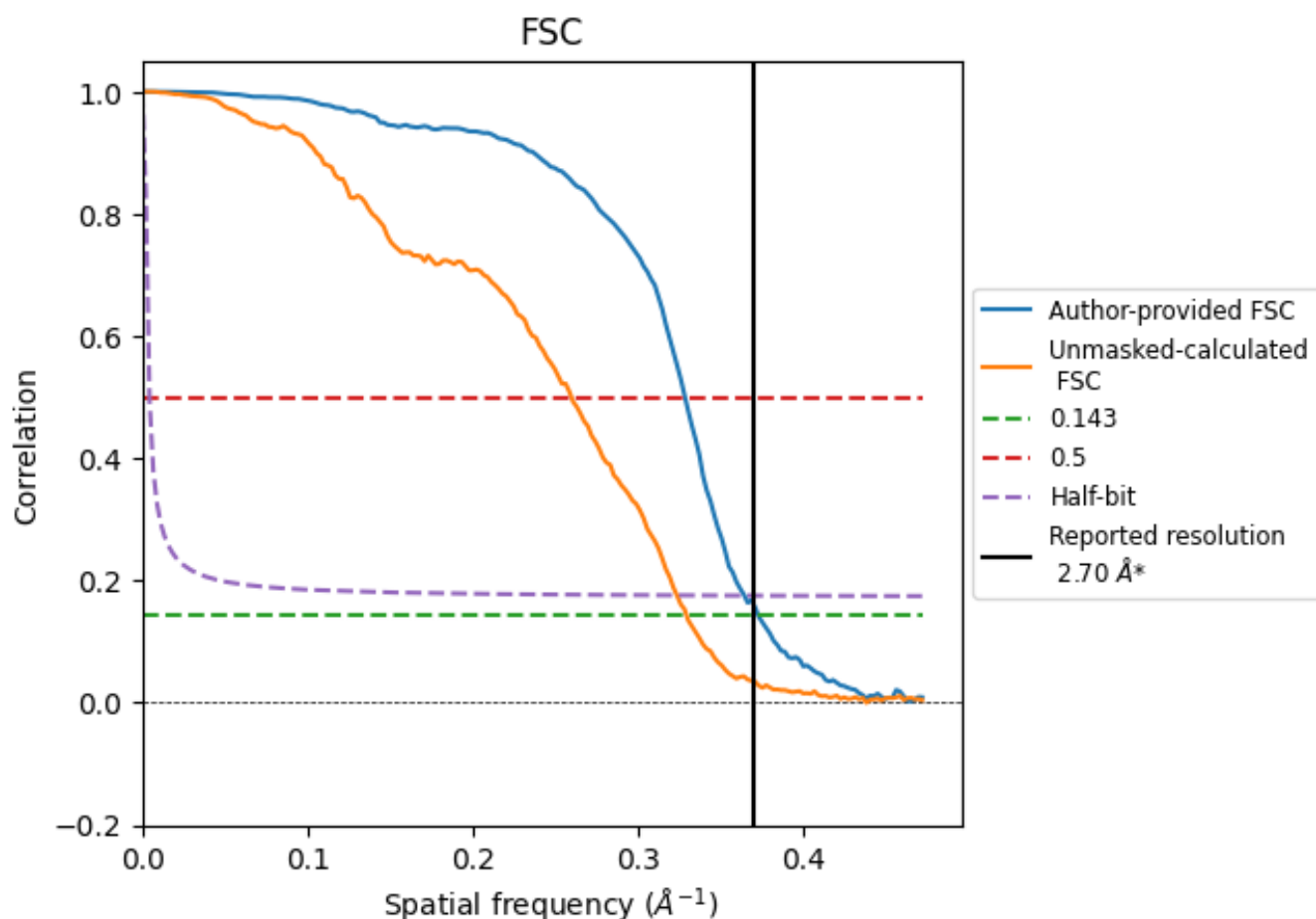


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

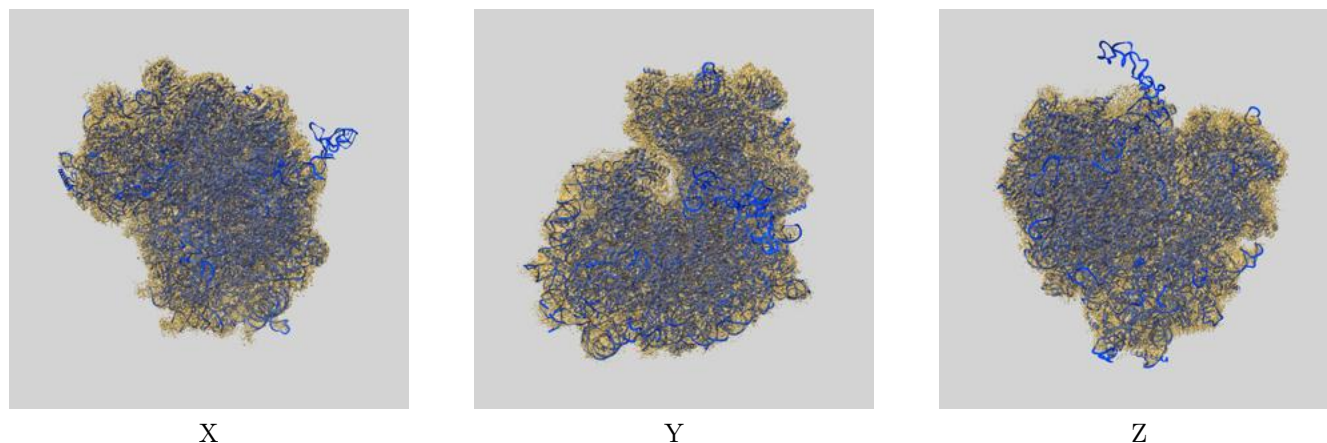
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.04	2.74
Unmasked-calculated*	3.03	3.85	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

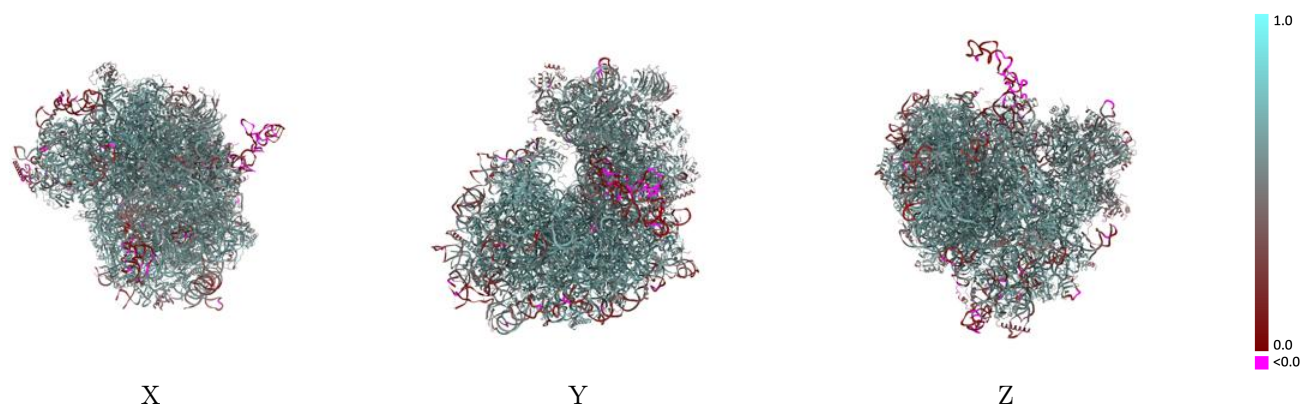
This section contains information regarding the fit between EMDB map EMD-33329 and PDB model 7XNX. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



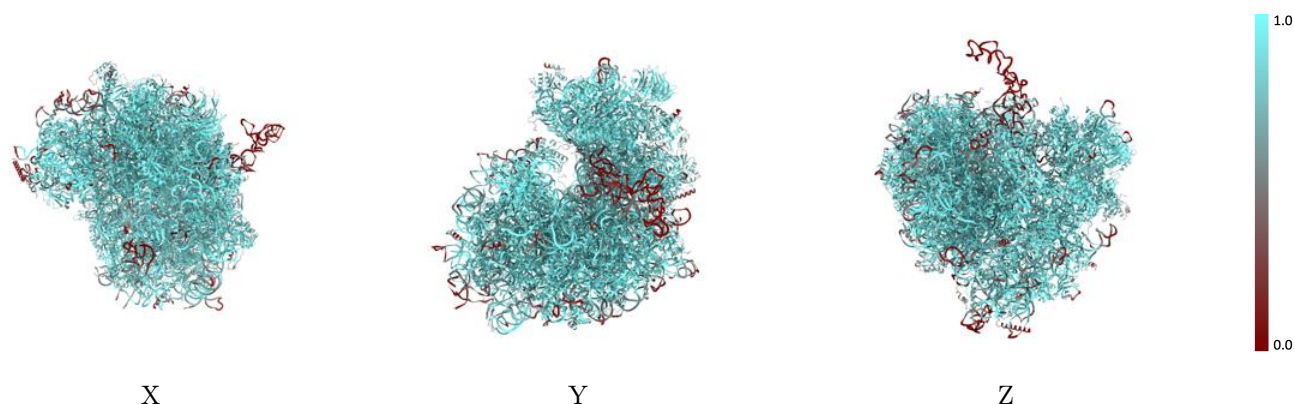
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



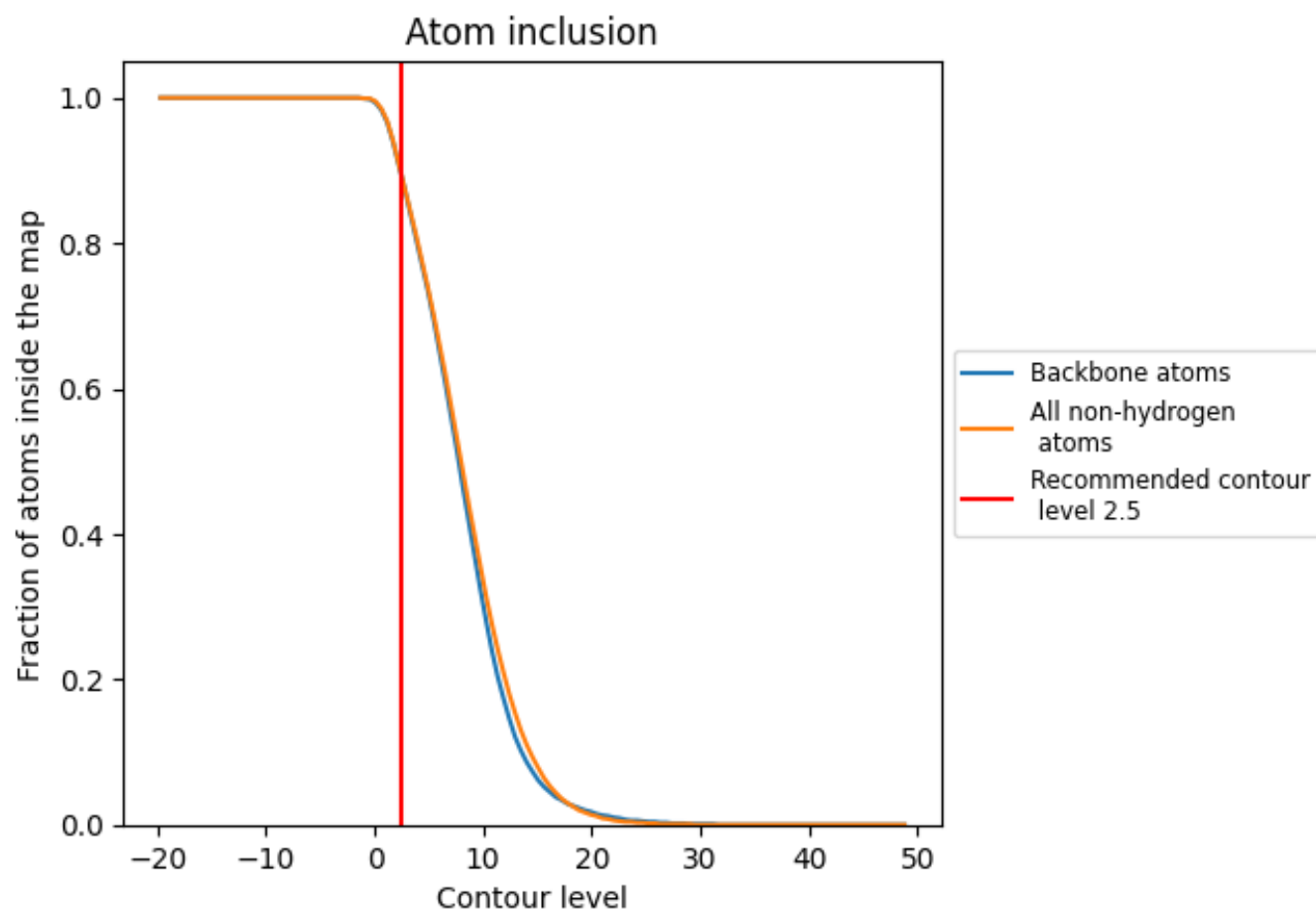
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.5800
CC	 0.3530	 0.3020
CE	 0.7000	 0.5000
L1	 0.8790	 0.5720
L2	 0.9870	 0.6430
L3	 0.9340	 0.6070
LA	 0.9810	 0.6740
LB	 0.9310	 0.6390
LC	 0.9360	 0.6380
LD	 0.8840	 0.6010
LE	 0.8790	 0.5910
LF	 0.9550	 0.6530
LG	 0.8360	 0.5730
LH	 0.9080	 0.6100
LI	 0.9420	 0.6350
LJ	 0.8190	 0.5520
LL	 0.8790	 0.5920
LM	 0.9120	 0.6020
LN	 0.9890	 0.6800
LO	 0.9470	 0.6490
LP	 0.9380	 0.6510
LQ	 0.9700	 0.6660
LR	 0.8510	 0.6000
LS	 0.9670	 0.6540
LT	 0.9200	 0.6230
LU	 0.7080	 0.5060
LV	 0.9570	 0.6520
LW	 0.5960	 0.4410
LX	 0.9300	 0.6350
LY	 0.8990	 0.6060
LZ	 0.9040	 0.6110
La	 0.9530	 0.6540
Lb	 0.7910	 0.5400
Lc	 0.9370	 0.6250
Ld	 0.8950	 0.6190



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Chain	Atom inclusion	Q-score
Le	 0.9620	 0.6530
Lf	 0.9700	 0.6590
Lg	 0.9140	 0.6220
Lh	 0.8900	 0.5990
Li	 0.9070	 0.5990
Lj	 0.9720	 0.6580
Lk	 0.7500	 0.5510
Ll	 0.9480	 0.6340
Lm	 0.9280	 0.6340
Ln	 0.9620	 0.6230
Lo	 0.9350	 0.6420
Lp	 0.9650	 0.6600
Lr	 0.9410	 0.6320
S2	 0.9120	 0.5780
SA	 0.9090	 0.5950
SB	 0.9140	 0.5880
SC	 0.9630	 0.6240
SD	 0.9350	 0.5380
SE	 0.9460	 0.5990
SF	 0.9370	 0.5560
SG	 0.8420	 0.5110
SH	 0.8060	 0.4950
SI	 0.8870	 0.5720
SJ	 0.9030	 0.5730
SK	 0.9080	 0.5160
SL	 0.9360	 0.6330
SM	 0.6560	 0.2980
SN	 0.9570	 0.6340
SO	 0.9470	 0.6090
SP	 0.8680	 0.4790
SQ	 0.9150	 0.5290
SR	 0.7960	 0.5340
SS	 0.8830	 0.4890
ST	 0.9140	 0.5330
SU	 0.8790	 0.4870
SV	 0.9260	 0.6000
SW	 0.9720	 0.6430
SX	 0.9580	 0.6240
SY	 0.9080	 0.5570
SZ	 0.8830	 0.5120
Sa	 0.9250	 0.6030
Sb	 0.8980	 0.5840

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Chain	Atom inclusion	Q-score
Sc	 0.8890	 0.5170
Sd	 0.9500	 0.5660
Se	 0.7810	 0.5200
Sf	 0.8140	 0.4610
Sg	 0.9100	 0.5050